Global Activity Report

Portuguese Nuclear Magnetic Resonance Network

2010-2012

For further information or additional copies of this report, please contact

Angelo M. Figueiredo or Eurico J. Cabrita

Dept. Quimica, Faculdade de Ciências e Tecnologia

Universidade Nova de Lisboa

Quinta da Torre, 2829 -516 CAPARICA

PORTUGAL

Or visit the website at:

http://ptnmr.dq.ua.pt/

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Foreword

About the Portuguese Nuclear Magnetic Resonance Network

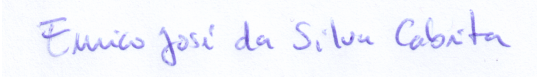
The Portuguese Nuclear Magnetic Resonance (PTNMR) network was created in 2005 with the support of the Portuguese Foundation for Science and Technology (FCT-MEC) in the frame of a national program (2003-2007) for acquisition and upgrading of scientific equipment. The main purpose is to endow the Portuguese research community with state-of-the art NMR equipment and to establish a national NMR hub to provide services in a spirit of partnership between all participating institutions. One of the objectives of the PTNMR is to promote collaboration between the several poles of the network, and to save funds by coordinating the re-equipment among all participating institutions, avoiding also undesirable duplication of equipment.

After the installation period (2007) the first two years of operation of the PTNMR (2008 and 2009) had no specific funding program. By the end of 2009, PTNMR activities were formally reported to FCT for evaluation. This evaluation considered scientific, operational and financial aspects such as: spectrometer usage, network activities (e.g. workshops, courses and other training activities), impact in post-graduate training (e.g. number of PhDs and post-docs), impact in research activity (e.g. number of research projects supported), and other scientific production indicators (e.g. publications, communications in conferences, etc) and operational costs (human resources and maintenance).

Together with the report to FCT-MEC, PTNMR presented also a proposal for the network activities and operation for the period 2010-2012 with a request for funding. The evaluation process led to the approval of the financial support of PTNMR by FCT-MEC and to the signature of a "contrato-programa" between all PTNMR partners and FCT-MEC for the period 2010-2012.

This documents reports the PTNMR network operation and activities performed during the period 2010-2012 under the “contrato-programa” signed with FCT-MEC.

Detailed information about the network and current and past activities can also be found in the network home page on the internet: http://ptnmr.dq.ua.pt.



Eurico J. Cabrita

PTNMR Network coordinator 2010-2012

Description

Objectives

The main objective of the PTNMR network is to provide to national researchers and their academic and industrial partners access to NMR spectrometers and techniques for liquids and solids. In this context, PTNMR offers services and scientific expertise in solution and solid state NMR that support national R&D initiatives.

Other general objectives of the PTNMR are: to ensure a stimulating research environment by promoting networking and training activities, to guarantee a continuous training at graduate and postgraduate level and to enhance opportunities for collaborative and multidisciplinary research on national and international levels.

PTNMR is organized and managed according to a policy agreed between all the partners and FCT-MEC that includes specific rules for the management and access to the equipment (Annex 1). In the context of the “contrato-programa” with FCT-MEC, all participating institutions share the same responsibilities:

- to manage the local NMR equipment;

- to provide access to national and international researchers;

- to provide services to the scientific community and industry in their areas of expertise;

- to promote training in the use of the technology and support local advanced training initiatives.

PTNMR Infrastructure and Equipment

The following institutions are part of the Portuguese NMR Network: Universidade de Aveiro (CICECO and QOPNA), Universidade de Coimbra through its Faculdade de Ciências e Tecnologia and the Center for Neuroscience and Cell Biology, Universidade Nova de Lisboa through its Faculdade de Ciências e Tecnologia, the Instituto de Tecnologia Química e Biológica-CERMAX, and the CENIMAT/I3N, Universidade Técnica de Lisboa through the Instituto Superior Técnico, Universidade da Madeira (CQM), Universidade do Minho and Universidade do Porto (Figure 1).

FIGURE 1 - Geographical distribution of PTNMR Infrastructure with identification of spectrometers by magnetic field strength.

The list of spectrometers spread across the country consist of:

- One 800 MHz NMR spectrometer - Bruker Avance II+ NMR spectrometer (ITQB-UNL) with solution and solid state capabilities.
- Two 600 MHz NMR spectrometers - one Bruker Avance II+ NMR spectrometer equipped with a cryoprobe (REQUIMTE-FCT-UNL), one Varian VNMRS600 600 MHz NMR spectrometer (CNC, Univ. Coimbra)
- Five 500 MHz NMR spectrometers - two Bruker Avance II+ NMR spectrometers 500 MHz (ITQB-UNL, IST-UTL), two Bruker Avance II NMR spectrometer 500 MHz (ITQB-UNL, Univ. Aveiro), one Varian Unity500 500 MHz NMR spectrometer (CNC-Univ. Coimbra).
- Eight 400 MHz NMR spectrometers - seven Bruker Avance II+ NMR spectrometers 400 MHz (Univ. Porto, Univ. Minho, FCT-Univ. Coimbra, IST-UTL, ITQB-UNL, REQUIMTE-FCT-UNL, Univ. Madeira), one wide bore SSNMR Bruker Avance III NMR spectrometer 400 MHz (Univ. Aveiro).
- Five 300 MHz NMR spectrometers - one Bruker Avance II+ NMR spectrometers 300 MHz (IST-UTL), one wide bore SSNMR Bruker Avance II+ NMR spectrometer 300 MHz equiped with a microimaging and a diffusion probe (CENIMAT-FCT-UNL), one wide bore SSNMR Tecmag (Redstone)/Bruker NMR spectrometer 300 MHz equiped with

static, MAS, DOR and stray-field imaging probes (IST-UTL), one Bruker Avance 300 MHz NMR spectrometer (Univ. Aveiro).

- An exhaustive list of all the equipment and accessories can be found at the PTNMR homepage in the internet (http://ptnmr.dq.ua.pt).

Management and user policy

The management structure consists of a General Network Coordinator, a Management Committee, a local Manager per unit, an International Advisory Board and a Project Evaluation Panel. The main duties/responsibility of the elements of this structure are briefly described here, a full description can be found in Annex 1.

Management Committee - chaired by the *General PTNMR Coordinator*, approves the annual financial budget and is responsible for the operation of the whole PTNMR network; coordinates the development of all NMR units keeping in mind the high levels of services offered to the Portuguese scientific community, and takes actions to implement the necessary improvements. The Management Committee must establish the rules for access to the Network facilities and coordinate the general activities so that a cost effective network is achieved. This Committee reviews annually the structure of user fees, the budget of each NMR unit, the proposed courses/seminars/conferences and submits reports to be compiled onto the Annual Report of the PTNMR network.

NMR Unit Manager - The NMR unit manager is responsible for the day-to-day operations in each partner institution. The manager is the liaison between the users and the Management Committee providing assistance, support and training to users and reporting directly to the PTNMR Coordinator. It is also the duty of the NMR unit manager to maintain a dedicated webpage of the Unit including a public updated calendar of spectrometer use and a list of equipment and services.

International Advisory Board - recognized experts of the international NMR community appointed by the Management Committee - provides comments, suggestions and recommendations on the efficiency of the operations, on the basis of report evaluation.

Project Evaluators Panel - Is responsible for the evaluation of project proposals for spectrometer use. Evaluates the proposals concerning scientific merit and adequacy of requested NMR time. The Management board is responsible for the designation of the specialists in the panel.

Spectrometer use is managed by the Unit manager according to three types of use:
- regular (direct decision by the Unit manager)
- project based (by recommendation of the Project Evaluators Panel)
- service to companies

Time management and allocation to users depends on the category of Spectrometer. PTNMR spectrometers are divided into two categories according to the Magnetic Field:

High Field Spectrometers (above 600 MHz)
Spectrometer use is managed in a monthly base with the following priority rule:
- 70 % of the total spectrometer is made available to external users

Low Field Spectrometers (below 600 MHz)
Spectrometer use is managed in a weekly base with the following general rule:
- 30 % of the total spectrometer time is made available to external users

Each Unit Manager is responsible for publishing the calendar of user time allocation on a weekly (low field spectrometers) or monthly (high field spectrometers) base as well as the general rules for spectrometer use and the forms for project proposals in their unit webpage.
User Project Proposals are send by the Unit Manager to the General Coordinator, that selects two specialists from the Project Evaluators Panel to review the proposal. The decision should be communicated to the Unit Manager and the User in no more than a week after receiving the proposal.

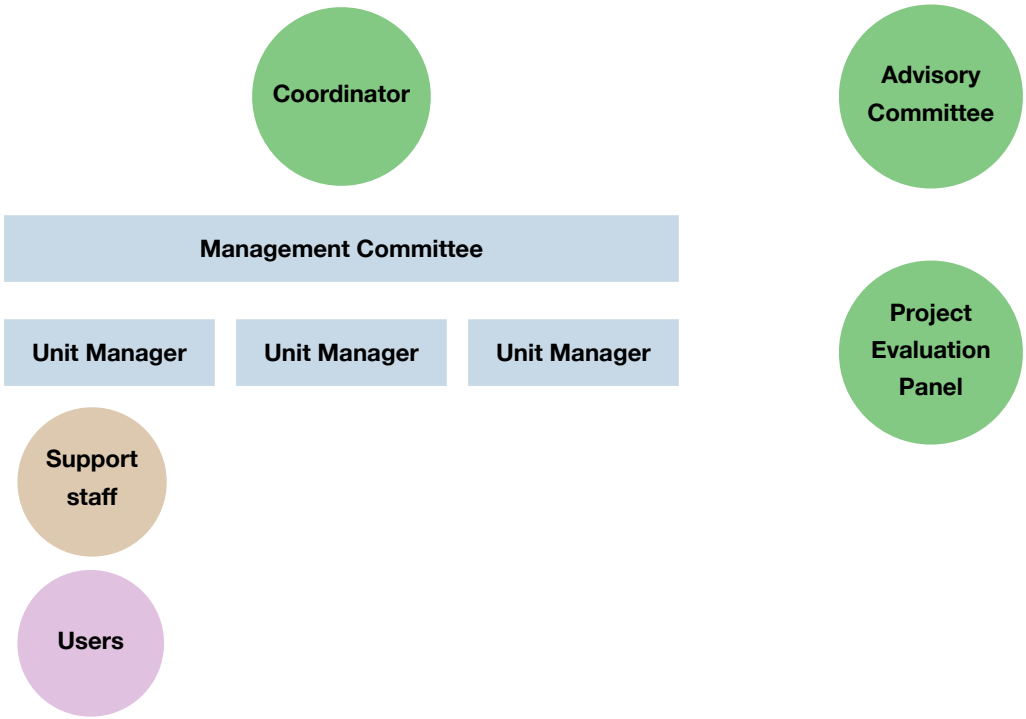


FIGURE 2 - Scheme of the management structure of the PTNMR network.

Main Research and Development Topics

The main policy of PTNMR Network is to conduct science and technology activities, fostering knowledge transfer and promoting the involvement of national and foreign researchers in RD&I projects in their areas of expertise. The RD&I activities comprise both fundamental aspects and projects with a strong applied component in multiple areas of intervention. Most of these leading activities are conducted in local Institutes and Faculties targeted to the real problems of local activities. Thus, the excellence of the research therein developed is a key factor for the success of policies aiming creation of leading industries in emergent areas of Life Sciences, Materials, Nanotechnologies and Nanosciences.

State of the art of the research being done in the PTNMR is organized according to the following main scientific topics:

1 - Structural Biology

The study of protein structure and dynamics is of paramount importance to develop practical strategies to create new biotechnological applications and new approaches to treating diseases. Solution and SSNMR are being used to obtain structural information in solution or solid state on macrobiomolecules such as proteins and nucleic acids.

2 - Material Sciences

NMR is being used to assist the development of novel nano- and micro-structured materials including organic-inorganic hybrids, multifunctional materials, ferroic ceramics and nanostructures allowing the study of structure-property (electrical, magnetic, optical and biological) relationships and the design of devices for information and communication technology.

3 - Small molecules (structure, dynamics and interaction)

NMR is an essential technology for determining not only molecular structure but also molecular interactions. NMR techniques are used to characterize the binding surfaces between small molecules and larger biomolecular targets, to screen small molecule libraries to define chemical toolboxes for drug design as used in the pharmaceutical industry.

4 - Metabonomics and Metabolomics

In metabolic and physiological studies, NMR is used as a tool for the discovery of new pathways, to guide metabolic engineering strategies in industrial microbes (fluxomics), and for unravelling the metabolic effects of disease and disease therapies. Lung cancer and pregnancy disorders are just two examples being studied within the PTNMR.

Network Activities

Network activities promoted by the PTNMR network are focused in two mains axes:
- Meetings and educational programs, such as courses, research training, workshops and conferences.
- Human mobility between different research groups in order to share knowledge/experience and to strengthen cooperation in terms of research projects.

The support of the network to these activities is done through promotion on its own website (http://ptnmr.dq.ua.pt/) and through financial support for the organization of seminars and courses with international recognized specialists in the NMR field. Mobility is fostered by supporting travel and accommodation expenses of researchers and/or students of the different centers that constitute the network for training activities or data acquisition on other centers of the network.

PTNMR is actively engaged in post-graduate education creating an international atmosphere nationwide, sponsoring and organizing a program of seminars and lectures, given by invited internationally recognized speakers. These are open to all scientific community. These seminars are crucial to expose the portuguese scientific community to new ideas, to stimulate the internationalization of the national NMR scientific community and to promote the image of the Portuguese science in the world.

The PTNMR network is also involved in international NMR activities, participating in major international and national NMR events, organizing conferences, workshops and courses.

Training activity within the PTNMR network is diverse, targeting different expertise levels, from introductory courses to advanced hands-on training.

Budget and funding

The PTNMR budget and income sources in the period 2010-2012 are resumed in Table 1.

Table 1 - Global PTNMR budget with description of income sources

	2010[a]		2011[b]		2012[b]		Total	
Income source	**k Eur.**	**%**	**k Eur.**	**%**	**k Eur.**	**%**	**k Eur.**	**%**
National Scientific Agency (FCT-MEC)	412.5	82	406.5	84	464.5	85	1283,5	83
Own income sources from Affiliated Centres and Research Institutes	91	18	84.4	16	85.1	15	260,5	17
TOTAL/year	**503.5**	**100**	**490.9**	**100**	**549.6**	**100**	**1544**	**100**

[a] 2010 values are those of the original "contrato-programa" with FCT-MEC. [b] The budget for 2011 and 2012 was revised after the first annual report to FCT-MEC. The revised values are presented.

PTNMR budget is organized in two major categories: Operational costs and Networking costs, each with different sub-categories as resumed in Table 2.

Table 2 - Global PTNMR budget allocated to Operational and Networking costs description of income sources (values in k Eur).

	2010[a]					2011[b]					2012[b]					Total
Category	**FCT-MEC**	**%**	**Co-financing**	**%**	**Total**	**FCT-MEC**	**%**	**Co-financing**	**%**	**Total**	**FCT-MEC**	**%**	**Co-financing**	**%**	**Total**	**Total**
Human Resources	154	30.6	0	0	154	156,5	31.9	5,5	1.1	162	208,5	37.9	5,9	1.1	214	**530,4**
Maintenance	130,8	26	34	6.8	164,8	126,5	25.8	28	5.7	154,5	129,3	23.5	25,6	4.7	154,9	**474,2**
Other operational costs	100,7	20	46	9.1	146,7	105	21.4	44,4	9	149,4	108,2	19.7	47,1	8.6	155,3	**451,4**
Total Operational costs/year	**385,5**	**77**	**80**	**15.9**	**465,5**	**388**	**79**	**77,9**	15.9	**465,9**	**446**	81.1	**78,6**	14.3	**524,6**	**1456**
Networking Activities	27	5.4	11	2.2	38,0	18,5	3.8	6,5	1.3	25,0	18,5	3.4	6,5	1.2	25,0	**88**
Total / year	**412,5**	**81.9**	**91**	**18.1**	**503,5**	**406,5**	**82.8**	**84,4**	**17.2**	**490,9**	**464,5**	**84.5**	**85,1**	**15.5**	**549,6**	**1544**

Units and Expertise

CENIMAT - FCT/Universidade Nova de Lisboa

Located at:
CENIMAT/I3N – Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa

Web-page:
http://www.cenimat.fct.unl.pt/services/laboratory-nuclear-magnetic-resonance-nmr-spectroscopy

Magnet:
Bruker AvanceII+ 300
7 T, wide bore, Ultrashielded
1H frequency: 300 MHz

Console:
Avance II+ ?????-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
Running Topsin2.1 on Linux

NMR probes:
??????????????????????

The main areas of NMR study at CENIMAT are basis on spectroscopic characterisation of molecular dynamic and structure in solids and complex fluids. Focusing on the conformational effects observed on micro and nano cellulosic fibers when spun from liquid crystalline solutions. Rheologic and diffusion properties are studied by NMR spectroscopy; flow and defect characterization of these systems under capilar extrusion by MRI. Those fibers are studied to be used as functional and responsive materials for blood and tissue oxygenation.
Other area of expertise is the study of the structure, order and dynamics of liquid crystalline systems: e.g. dendrimers and Elastomers (LCE) and micro nano fibers prepared from cellulosic materials. The experimental results provide a basis for theoretical simulation.
The research pole is one of the main ones devoted to the study of Rheo-NMR of complex fluids in Portugal particularly the characterization of shear induced textures in complex fluids using Rheo-NMR Techniques. Associated with that diffusion studies are equally performed for studies on ionic diffusion in semi-conductive ion jelly systems by high power pulsed field gradients.

CERMAX - ITQB/Universidade Nova de Lisboa

Located at:
CERMAX, Centro de Ressonancia Magnetica Antonio Xavier, ITQB, Instituto de Tecnologia Quimica e Biologica – Universidade Nova de Lisboa

Web-page:
http://cermax.itqb.unl.pt/site/

Magnet:
Bruker AvanceII+ 800
18.8 T Ultra-Shield Plus
1H frequency: 800 MHz

Console:
4-channel digital AQS/2 Bruker Avance II+
Gradient: GRASP IIP
Temperature controlled BCU-05
HR-MAS control unit
Running Topsin2.1 on Linux

NMR probes:
5 mm inverse detection QXI (1H, 13C, 15N, 31P)
5 mm inverse detection TXI (1H, 13C, 15N)
5 mm BBI-Z, inverse broadband probe with Z-gradient coil tunable from 31P to 109Ag
10 mm direct detection QNP (auto-switchable quad nucleus probe for obs 1H, 13C, 31P and 19F)
5 mm BBO two channel (1H, observe channel X-nucleus covers frequency range from 31P to 109Ag)

For Solid State:
4 mm HR-MAS (1H, 13C, 15N)
3.2 mm Tri-gamma H/X/Y CP MAS probe
2.5 mm Tri-gamma H/X/Y CP MAS probe

3.2 mm Low-gamma between 49Ti amd 23Na CP MAS probe

Bruker Avance 800

Magnet:
Bruker AvanceIII 500
11.7 T, Ultra-Shield
1H frequency: 500 MHz

Console:
2-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
HR-MAS control unit
Running Topsin2.1 on Linux

NMR probes:
5 mm inverse detection QXI (1H, 13C, 15N, 31P)
10 mm QNP (1H, 19F, 13C, 31P)

For Solid State:
4 mm HR-MAS (1H, 13C, 15N)

Bruker Avance 500

Magnet:
Bruker AvanceII 500
11.7 T Ultrashielded plus
1H frequency: 500 MHz

Console:
2-channel digital
Gradient: GREAT 3/10
Temperature controlled BCU-05
Running Topsin2.0 on Linux

NMR probes:
10 mm QNP (1H, 19F, 13C, 31P)
5 mm dual probe for 1H and 13C
5 mm selective SEX probe
10 mm selective SEXNa
10 mm TXO-F/P
5 mm BBI-Z, inverse broadband probe with Z-gradient coil tunable from 31P to 109Ag

Bruker Avance 500

Magnet:
Bruker AvanceIII 400
9.4 T, Ultra-Shield Plus
1H frequency: 400 MHz

Console:
1-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
Running Topsin2.1 on Linux
Auto-sampler

NMR probes:
5 mm BBI(F)-Z, broad band for decoupling X nuclei between 31P to 97Mo
10 mm BBO-Z LR for direct observation of low frequency nuclei in the range from 39K to 41K
10 mm and 5 mm BBO two channel (1H, observe channel X-nucleus covers frequency range from 31P to 109Ag)

Bruker AvanceIII 400 with autosampler

Magnet:
Bruker DRX 300
7 T, narrow bore
1H frequency: 300 MHz

Console:
DRX console 2-channel digital
Gradient: GREAT 1/10
Temperature controlled BCU-05
Running Topsin1.3 on Linux

NMR probes:
5 mm BBI-Z, inverse broadband probe with Z-gradient coil tunable from 31P to 109Ag

Bruker DRX 300

The research at CERMAX has been focused on *in vivo* NMR (Helena Santos) to investigate cell metabolism and regulation. The H. Santos Group has pioneered the use of in vivo NMR techniques in Portugal to study metabolism of lactic acid bacteria and brain cells. Their expertise covers structural elucidation, protein dynamics and the discovery of new metabolic pathways. Similarly, the group of Ana Neves is dedicated to the study of metabolic and transcriptional regulation of sugar metabolism in lactic acid bacteria. Ana Rute has engaged on the application of in vivo NMR to probe biological processes directly in living cells. Through this effort she has gained substantial expertise in metabolite profiling and metabolic elucidation using NMR.
Taking advantage of the NMR large scale facility at the institute the groups of David Turner and Ricardo Louro study paramagnetic systems and haemproteins in terms of conformational changes that are couple to electron and proton transfer. Associated with the problematic of conformational change the groups of Manolis Matzapetakis and Pedro Lamosa are focus on structural characterisation: protein structure determination, dynamics and protein-protein interactions using fast acquisition and automated methods. Other area of NMR knowledge is on the study of molecular interactions. The group of Patrick Groves is focus on ligand binding protein methods that define molecular interactions of small molecules or ligands in the presence of biomolecules. Tranfer-NOESY techniques coupled with STD (saturation transfer difference) and DOSY are used to screen small molecule libraries (pharmaceutical applications) and to investigate specific ligands (biochemical applications).
The miscellany of the NMR use at the CERMAX also covers the structural identification of mainly organometallic complexes, that act as catalysts, potential pharmaceuticals, namely anti-tumoral drugs, as well as the identification of reaction products, intermediates and mechanisms involved in the catalytic reactions (Carlos Romao).

CICECO - Universidade de Aveiro

Located at:
NMR Lab – Chemistry Department, Universidade de Aveiro

Web-page:
http://www.ua.pt/dq/PageText.aspx?id=7526

Magnet:
Bruker Avance 300
7.1 T, narrow bore
1H frequency: 300 MHz

Console:
3-channel digital AQS/2 Bruker Avance II
Gradient: GREAT Z-Gradient
Temperature controlled

NMR probes:
QNP 5 mm (1H; 13C; 19F; 31P)
Inverse detected probe, triple tuned probe; X=broadband; Y=31P)
10 mm Broadband (31P-103Rb)

Bruker Avance 300

Magnet:
Bruker Avance 400
9.4 T, wide bore - ultrashielded
1H frequency: 400 MHz

Console:
3-channel digital AQS/2 Bruker Avance II
Gradient: GREAT Z-Gradient
Temperature controlled

NMR probes:
CP/MAS 2.5 mm
CP/MAS 4 mm
CP/MAS 4 mm for low γ nuclei
MAS 4mm – 1H CRAMPS
CP/MAS 7 mm
MAS 7 mm triple resonance
1 probe wide-line multi nuclei

Bruker Avance 400

Magnet:
Bruker Avance 500
11.75 T, wide bore - ultrashielded
1H frequency: 500 MHz

Console:
3-channel digital AQS/2 Bruker Avance II
Gradient: GREAT Z-Gradient
Temperature controlled

NMR probes:
CP-MAS 2.5 mm and 4 mm (for solids)
Complete LC-NMR system
QNP 5 mm (1H, 13C, 19F, 31P) and inverse detected (broadband); HR-MAS

Bruker Avance 500

From 1988 the NMR unit held in Aveiro has been pioneer in the methodological development and applications of NMR in solid state, particularly for the study of quadrupolar nuclei. Some of the techniques developed are basis on 2H exchange spectroscopy, quadrupole nutation and double rotation, and satellite transition spectroscopy (Joao Rocha Group). Using high-resolution NMR methods for solids, 1H (CRAMPS) and quadropular spins have been applied in Portugal for the study of small molecules and inorganic-organic hybrid materials (Luis Mafra Group).
Similarly, NMR in liquids has been used as the main tool for comprehensive characterisation of chemical structure, conformations and configurations of synthetic and natural molecules. Mainly, polyphenolics and nitrogen heterocyclic compounds; tetrapyrrolic macrocycles and polyphenolic compounds isolated from red wines (Artur Silva Group).
The diversity of NMR techniques in Aveiro also covers metabolomics analysis. With state of the art equipment, analytical strategies based on high resolution NMR (liquids, HRMAS, hyphenated NMR, LipoProfiling for lipoprotein analysis) and MS technologies (namely UPLC-MS and targeted LC-MS for lipoprofiling) have been applied in metabonomic analysis of human biofluids and biological tissues for diagnosis, prognosis and monitoring of diseases (Ana Gil and Iola Duarte Groups).
Structural bioinorganic chemistry by NMR spectroscopy has been also studied by Brian Goodfellow Group, mainly small metalloproteins containing simple Fe-S centres. By replacing the native Fe by diamagnetic metals, such as Zn and Cd the structure of these proteins can be obtained and by using paramagnetic derivatives, such as Ni, the electronic distribution at the active site have been probed using residual dipolar coupling and pseudocontact shifts.

CNC - Universidade de Coimbra

Located at:
LabRMN – Center for Neuroscince and Cell Biology – Universidade de Coimbra

Web-page:
http://www.cnbc.pt/services/rmn_2.asp

Magnet:
Varian VNMRS600
14.1 T, narrow bore
1H frequency: 600 MHz

Console:
3-channel digital AQS/2 Bruker Avance II
Gradient: GREAT Z-Gradient
MAS control unit
Temperature controlled

NMR probes:
5 mm inverse detected triple resonance 1H{13C/15N}
5 mm direct detection broad band (31P-15N)
3 mm triple resonance inverse detected
3 mm broad band (31P-109Ag)
4 mm nanoprobe (HR-MAS)

Varian VNMRS 600

Magnet:
Varian Unity500
11.74 T, two channels
1H frequency: 500 MHz

Console:
3-channel digital AQS/2 Bruker Avance II
Gradient: GREAT Z-Gradient
MAS control unit
Temperature controlled

NMR probes:
5 mm inverse detected triple resonance 1H{13C/15N}
5 mm direct detection broad band (31P-15N)
10 mm direct detection broad band (31P-15N)
10 mm low frequency (15-50 MHz)

Varian Unity 500

The NMR unit is focused in two main areas: inorganic complexes for medical diagnosis, MRI and molecular imaging and metabolic fluxes.

The studies for medical diagnosis imaging include design, development and physico-chemical evaluation of metal based nanoparticles and small metal chelate agents for multimodal targeted medical imaging agents, followed by in vitro and animal model evaluation using MRI and nuclear imaging techniques (Carlos Geraldes Group).

Similarly, Margarida Castro Group is interested on the design and study of inorganic compounds as drugs for medical therapy (Li+ and bipolar disorder; vanadium complexes as oral insulin-mimetic agents). Her Group has been focus on the study of the effects of inorganic compounds on cell transport metabolism using metal (eg. 7Li, 23Na) through 31P and 13C NMR (with isotopomer analysis of 13C-enriched metabolites).

Investigation of glucose, protein and lipid homeostasis are studied in human subjects, in animal models of human diseases, and in isolated perfused animal organs by the John Jones Group. Their studies explore the use of 13C NMR isotopomer analysis of 13C-enriched metabolites from perfused organs, plasma glucose and urinary metabolites by direct and indirect detection methods. Similarly, 2H NMR analysis of metabolite positional is also performed in human plasma and urinary metabolites.

CQM - Universidade da Madeira

Located at:
Centro de Quimica da Madeira – Universidade da Madeira

Web-page:
http://cqm.uma.pt/nmr/

Magnet:
Bruker Avancell+ 400
9.4 T, Ultrashielded
1H frequency: 400 MHz

Console:
Avance II+ 2-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
Running Topsin2.1 on Linux
NMR case – autosampler

NMR probes:
5 mm BBO, two channel (1H, observe channel X-nucleus covers frequency range from 31P to 109Ag).

Bruker Avancell+ 400 MHz.

The main research topics at CQM are taken on two main areas: dendrimers and molecular wires. The main goal is the preparation and characterization of new types of molecular materials (dendrimers) and polymeric metal and

non-metal containing systems) with enhanced electronic and biomedical properties.

Together with other techniques (like MS), liquid NMR is used as a routine tool for the structural characterisation of the prepared compounds. Behind the common and typical NMR nucleus (1H and 13C), 31P is one of the most important nucleus used for the study of the electronic influence and the geometrical arrange of co-ligands around the metal centres. Overall NMR is used as a major tool for the comprehensive characterisation of the chemical structure of synthetic and natural molecules.

CQ - Universidade do Minho

Located at:
Centro de Quimica - Universidade do Minho

Web-page:
http://www.cq.uminho.pt/Default.aspx?tabid=11&pageid=211&lang=pt-PT

Magnet:
Bruker AvanceIII 400
9.4 T, Ultrashielded
1H frequency: 400 MHz

Console:
Avance III 3-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
Running Topsin2.1 on Linux

FCT - DQ - Universidade de Coimbra

Located at:
Laboratorio de Ressonancia Magnetica Nuclear – Centro de Quimica de Coimbra - Universidade de Coimbra

Web-page:
http://nmrccc.uc.pt/

Magnet:
Bruker AvanceIII 400
9.4 T, Ultrashielded
1H frequency: 400 MHz

Console:
Avance III 3-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
Running Topsin2.1 on Linux
NMR case – autosampler

NMR probes:
5 mm BBO, two channel (1H, observe channel X-nucleus covers frequency range from 31P to 109Ag)
5 mm inverse detection TXI (1H, 13C, 15N)

IST - Universidade Técnica de Lisboa

Located at:
Centro de Quimica Estrutural- Instituto Supeior Tecnico - Universidade Tecnica de Lisboa

Web-page:
http://cqe.ist.utl.pt/networks/nmr/nmr_equipment.php

Magnet:
Bruker AvanceII+ 300
7 T, Ultrashielded
1H frequency: 300 MHz

Console:
Avance II+ 2-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
Running Topsin2.1 on Linux

NMR probes:
5 mm broad band BBFO

Bruker Avance II+ 300 MHz

Magnet:
Bruker AvanceII+ 400
9.4 T, Ultrashielded
1H frequency: 400 MHz

Console:
Avance II+ 2-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
Running Topsin2.1 on Linux

NMR probes:
5 mm broad band BBFO

Bruker Avance II+ 400 MHz

Magnet:
Bruker AvanceII+ 500
11.7 T, Ultra-Shield
1H frequency: 500 MHz

Console:
3-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
HR-MAS control unit
Running Topsin2.1 on Linux

NMR probes:
3, 5 and 10 mm BBFO
5 mm inverse detection TXI (1H, 13C, 15N)

For Solid State:
4 mm HR-MAS (1H, 13C, 15N)

Bruker Avance II+ 500 MHz

The use of NMR at CQE is mainly on structural elucidation of small peptides and polymers by solution NMR. This support to in-house research groups (synthesis and catalysis) also explores the use of the NMR technique to diffusion experiments mainly in organometallics and NMR spin transfer techniques in ligand-host interactions. Concomitant with liquid state NMR development, the unit provide application insights on the use of magic angle spinning NMR to gels and cells.

REQUIMTE - FCT/Universidade Nova de Lisboa

Located at:
Chemistry Department – Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa

Web-page:
http://www2.dq.fct.unl.pt/servicos/rmn/LABRMN/Home.html

Magnet:
Bruker Avance II+ 600
14.1 T, narrow bore
1H frequency: 600 MHz

Console:
4-channel digital AQS/2 Bruker Avance II+
Gradient: GREAT Z-Gradient

Temperature controlled BCU-05

NMR probes:
Cryoprobe TCI (1H, 13C, 15N)
5 mm QNP (1H, 19F, 13C, 31P)

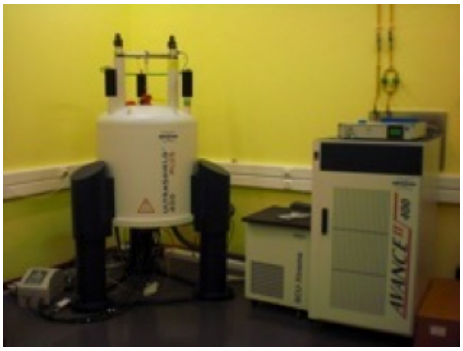
Bruker Avance II+ 600 equipped with a TCI cryoprobe

Magnet:
Bruker Avance II+ 400
9.4 T, narrow bore
1H frequency: 400 MHz

Console:
3-channel digital AQS/2 Bruker Avance II+
Gradient: GREAT Z-Gradient
HR-MAS control unit
Temperature controlled BCU-05

NMR probes:
5 mm TXI (1H, 13C, 15N)

For Solid State:
4 mm HR-MAS (1H, 13C, 15N)



Bruker Avance II+ 400

Magnet:
Bruker AvanceIII 400
9.4 T, narrow bore
1H frequency: 400 MHz

Console:
Nanobay, 2-channel digital
Automatic sampler NMR case

NMR probes:
5 mm QNP (1H, 19F, 13C, 31P)
5 mm BBI-Z

Bruker Nanobay 400

The current work develop on the NMR unit is focused mainly in the determination of protein structures and dynamics of a variety of molecules of chemical and biological interest.

The research groups hosted at REQUIMTE-FCT have a long tradition of application of NMR techniques to the study of metalloproteins, focusing on paramagnetic effects (Sofia Pauleta, Isabel Moura, Jose Moura, Carlos Salgueiro and Anjos Macedo). Case studies are rubredoxin, heme, iron-sulfur proteins and metalloenzymes.

While many of the projects involve the use of NMR spectroscopy in liquids as a major technique the group of Eurico Cabrita is involved on the application and development of NMR techniques to study intermolecular interactions in chemical and biological systems. His group combines NMR spectroscopy and organic synthesis with molecular modelling to study a wide range of chemical and biochemical reaction mechanisms.

Universidade do Porto

Located at:
REQUIMTE – Centro de Investigacao em Quimica, Departamento de Engenharia Quimica da FEUP, Instituto

de Ciencias Biomedicas Abel Salazar - Universidade do Porto

Web-page:
http://www.cemup.up.pt/cemup3lrmn.html

Magnet:
Bruker AvanceIII 400
9.4 T, Ultrashielded
1H frequency: 400 MHz

Console:
Avance III 3-channel digital
Gradient: GRASP IIP
Temperature controlled BCU-05
Running Topsin2.1 on Linux

NMR probes:
5 mm broad band BB-1H-D
5 mm inverse detected triple resonance 1H-BB-D

Spectrometer Use

To better present the spectrometer use within the PTNMR network, the percentage of annual time used on the spectrometers was calculated and grouped into two categories: High-field spectrometers (800 MHz (CERMAX-ITQB), 600 MHz (REQUIMTE-FCT/UNL) and 600 MHz (CNC - UCoimbra)) and low-field spectrometers (bellow 600 MHz).
Figures 1 and 2 show the percentage of the annual time used according to the magnetic field classification for the years 2010, 2011 and 2012.

Figure 1 - Total occupancy time (annual basis) of High-Field Spectrometers

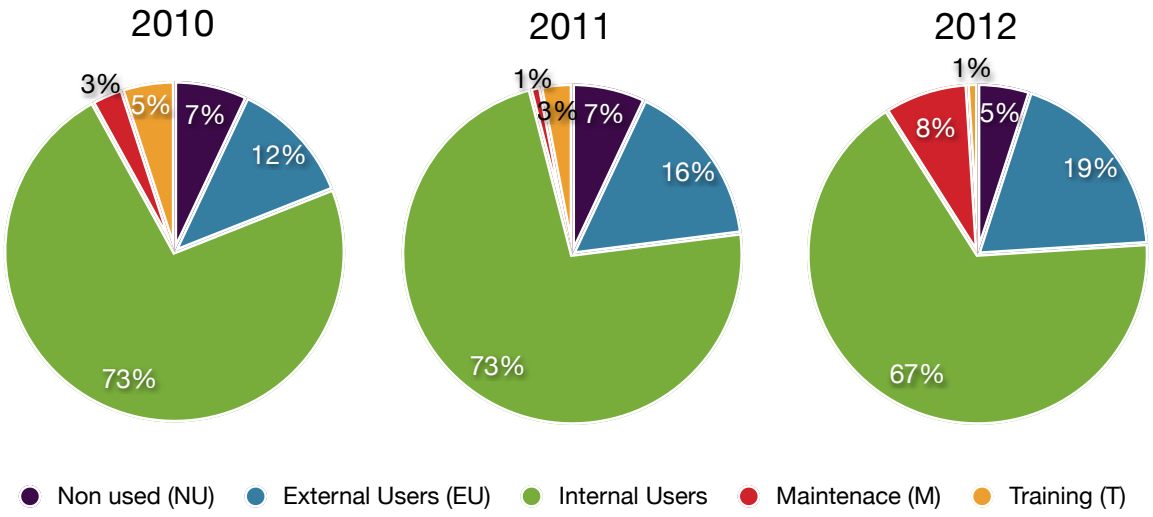
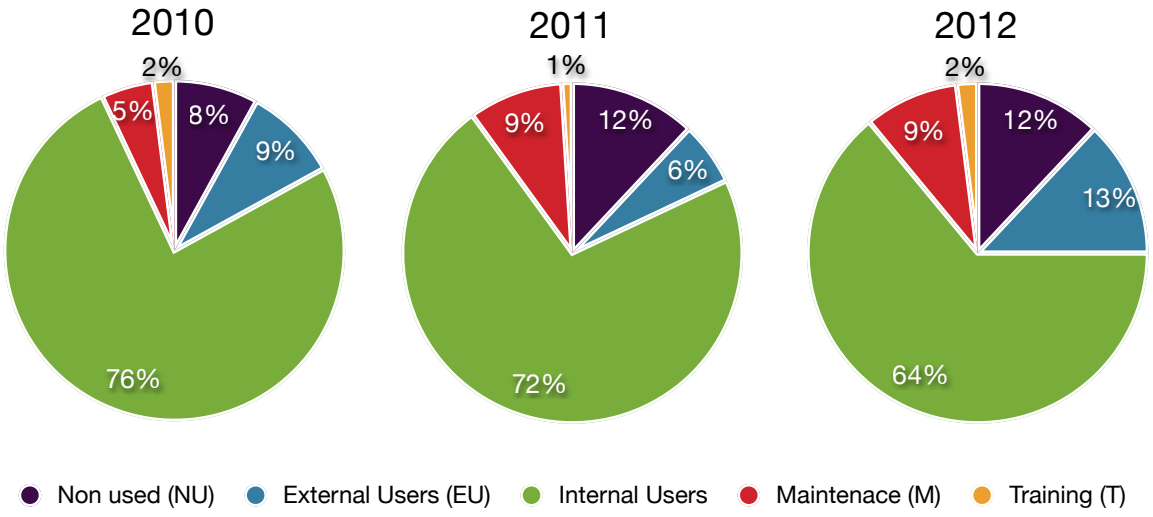


Figure 2 - Total occupancy time (annual basis) of Low-Field Spectrometers



As shown in Figures 1 and 2, the spectrometers from the PTNMR Network have been highly used in the period 2010 - 2012. On average the spectrometers were used 90% of the total annual time available.

One of the main purposes of the PTNMR Network is to provide external services to academic entities outside the network and to the private sector. For all the spectrometers the graphs shown in figures 1 and 2 reveal a common trend of increasing use by external users over the 3 years under report.
External academic users, searching for more specialized NMR services were mainly responsible for the external use of the labs equipped with high-magnetic fields such as, the 800 MHz located at ITQB-UNL and the 600 MHz on REQUIMTE/FCT-UNL and CNC-Univ. de Coimbra.

Relative to the low-field NMR spectrometers, this equipment is used more routinely for analysis and most of the use in 2010 and 2011 was to assure internal users routine analysis. However it is noticed a substantial increase on the percentage of external users of the low field spectrometers in 2012 face to 2010 and 2011. This increase is mainly due to the establishment of the PTNMR network as a routine service provider to other academic entities such as Universidade do Algarve and Universidade de Évora, that are the academic entities that most use the PTNMR services.

Regarding services to the private and industrial sector, during this period PTNMR has also provided regular analysis service for companies, such as Hovione, Bial and Sopac. In 2012, there was a significant increase in the number of requests from private companies. This increase reflects the efforts of the PTNMR network in advertising and stimulating the use of its services by private companies (e.g. the workshop NMR and Industry held in 2011).

Activities and Events

This section summarizes the PTNMR activity concerning training, organization of meetings and conferences and other events sponsored or supported by PTNMR.

2010

March

PTNMR Conference - Protein-Protein interactions and Protein folding

The national NMR network (PTNMR) in collaboration with the British Council has sponsored this event dedicated to the study of protein interactions and protein folding. The event taken on FCT-UNL (Caparica Campus) from 29th to 31st of March provided a unique forum for discussion of NMR methods applied to biomolecular systems. The conference was focus on recent developments in the field, with sessions and discussions devoted to some of the most exciting and topical aspects of biomolecular NMR. The conference provided an ideal platform for an interdisciplinary exchange of ideas.

PTNMR Course - 1st Hands on Course on Ligand based NMR interaction studies

Covering practical aspects of protein-ligand binding by NMR spectroscopy the course was intended for students and technicians in their studies. The aim of the course was to elucidate molecular interactions of small molecules or ligands in the presence of biomolecules. The course organised by the NMR group of REQUIMTE/FCT-UNL in conjunction with ITQB/UNL was held in Caparica Campus between 15th and 18th MarchThe topics covered during the course were diffusion NMR (DOSY), saturation transfer difference (STD) and transfer nuclear Overhauser effect spectroscopy (TR-NOESY). The course was intended to have theoretical sessions in the morning coupled with practical sessions in the afternoons enabling students to interact with spectrometers and acquire/analyze their own data.

The methods taught during the course were planned to be useful not only for research purpose on academia but also to industry, covering screening of small molecule libraries (pharmaceutical applications) and to investigate specific ligands (biochemical applications).

PTNMR Seminar – Prof. Jesus J Barbero – CIB/CSIC

Prof. Jiménez Barbero from Centro de Investigaciones Biologicas, CSIC, Madrid, Spain was invited by the NMR unit REQUIMTE-FCT-UNL (Caparica Campus) to give a lecturer on the development of NMR methodologies to the study of conformational and dynamical chances for the molecular recognition processes. In particular, he have paid attention to the physic-chemical origin of the interaction between carbohydrates and proteins, with special emphasis in the relative role of sugar-aromatic stacking interactions. This methodology has been applied to different carbohydrate molecular complexes of wild type and mutant lectins, glycosidases, and to the elucidation of the structure of other protein receptors of biomedical interest.

PTNMR Seminar – Prof. Beat H. Meier – ETH Zurich

The CICECO - Univ. Aveiro, NMR unit have invited Prof. B. Meier for a seminar under the topic of solid-state NMR. The meeting provided a forum for students and scientists from diverse experimental and theoretical backgrounds to discuss and explore new techniques to the study of biopolymers.

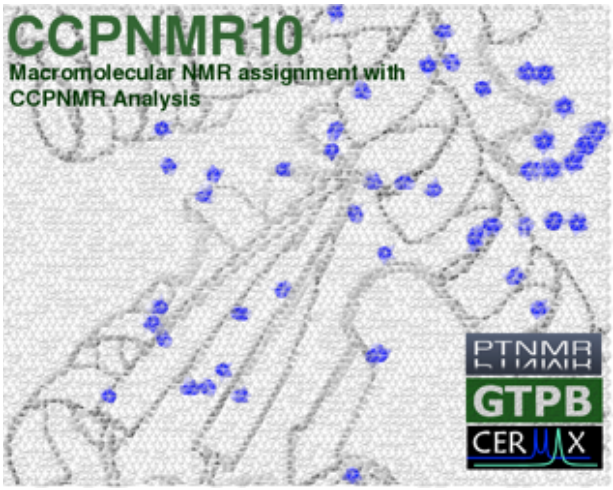
Prof. B. Meier is a well-known scientist on the development of new methods and the improvement on existing pulse sequences in solid-state NMR, with particular emphasis on polarization-transfer techniques, the refinement of the theoretical concepts for the description of spin systems under time-dependent Hamiltonians as well as numerical simulations and the study of local ordering phenomena in macroscopically disordered systems, e.g. glasses, amorphous synthetic polymers, biopolymers and polymerblends using NMR techniques.

June

PTNMR Sponsored Course - Macromolecular NMR assignment with CCPNMR Analysis

This course sponsored by the PTNMR between 31st of May and 4th of June at Instituto Gulbenkian de Ciencia (Oeiras) with the co-participation of ITQB/CERMAX was directed to the Portuguese NMR community for best practices in NMR and related areas (http://ptnmr.dq.ua.pt/index.php/network/activities/93-ccpnmr10).

The program included one day of introduction and theory of NMR, followed by 3 days of hands on tutorials on the use of the CCPNMR software package for the analysis of NMR spectra used in sequential assignment and solution structure determination. The final part was focus on describe protocols for structure determination and protein-protein interactions and in addition, the introducing of the eNMR European project as a future network that will offer a lot of functionalities to the biomolecular NMR community.



Poster layout of the CCPNMR Course

July

PTNMR Sponsored Course - IV Hands-on Course: From Proteomics to Proteins

Biomolecular NMR lecture module in the IV Hands on Course between 11th to 16th July. The aim was to provide basic knowledge about fundamentals on NMR spectroscopy for biomolecular sciences.

September

PTNMR Conference - V GERMN Biennale Meeting, II Iberian NMR Meeting

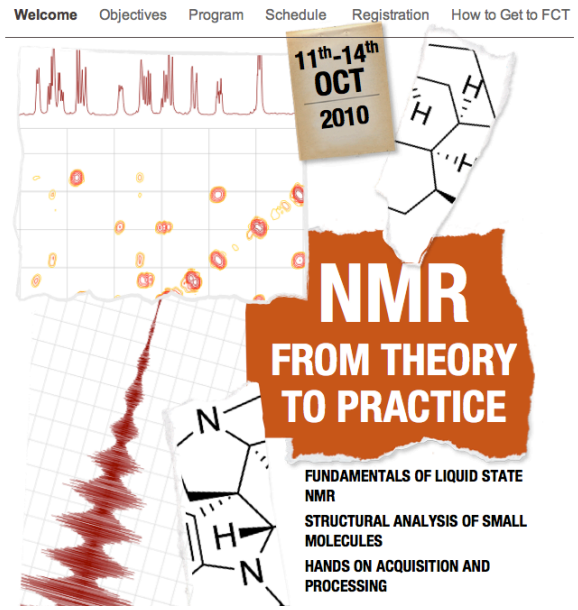
From 26th to 29th September, Bilbao hosted the important Iberian NMR meeting. This was a friendly meeting between Portuguese and Spanish NMR community showing the best of what has been done in Iberia during 2010.

October

PTNMR Course - NMR course from Theory to Practice

The course organised by the REQUIMTE/DQ/FCT-UNL NMR unit team between 11th and 14th October (http://www.dq.fct.unl.pt/nmrcourses/IntroNMR) covered basic theory of NMR spectroscopy combined with practical aspects of NMR acquisition and processing. This pioneer course counted with a large number of PhD, Post-Docs and Master students from Portuguese academia, for which the PTNMR network has fully supported travel and accommodation expenses for students outside Lisbon.

Standard 1D and 2D NMR techniques were employed by the students for structural analysis. During the course the students were able to interact with the spectrometer and analyze their own data.



Layout of the homepage of the course NMR:from theory to practice (http://www.dq.fct.unl.pt/nmrcourses/IntroNMR)

PTNMR Conference - NMR & Industry (Workshop)

The event held in CICECO, Aveiro (22nd October) was dedicated to show the potentialities of NMR and though the PTNMR network to the Industry. The workshop was announced to 700 businesses with the aim to present the national NMR network and show some practical examples of the NMR to solve common issues on industry, such as identification, characterization of compounds.

December

PTNMR Course - School on Modern Methods of Structure Elucidation

The course organised by IST-UTL Lisbon was focus on different spectroscopic techniques essential for structural elucidation. Topics covered range from solid state NMR and EPR spectroscopy to X-ray diffraction and mass spectrometry. The course provided a possibility to all participants to get hands-on training with equipment and present their scientific results during the flash presentation session. The school included theoretical sessions, provided by recognised specialists in the field, practical sessions and demonstrations of the equipment.

School on Modern Methods of Structure Elucidation held in the NMR unit at IST-UTL (http://cqe.ist.utl.pt/events/mmse2010/)

2011

February

PTNMR Seminar – Prof. Ivano Bertini – CERM, Florence

Prof. Ivano Bertini from CERM, Universita degli Studi di Firenze was invited to give a seminar at the Chemistry Department of REQUIMTE/FCT/UNL under the title: NMR: a flagship in moving the frontiers of biological science.

April

PTNMR Sponsored Conference - IYC 2011

Commemorating the international year of chemistry, Dr. Luis Mafra from CICECO/Universidade de Aveiro was invited to give a talk at the Chemistry Department of REQUIMTE/FCT/UNL under the title: Solid-state NMR methods applied to pharmaceuticals.

Reach out Activities - ExpoFCT

29th April – ExpoFCT, open day initiative by the NMR group at REQUIMTE/FCT-UNL for schools across Lisbon metropolitan area to present and exhibit the NMR science performed nationwide.

May

PTNMR Sponsored Conference – 2nd SMARTER Crystallography Workshop

This international workshop organised by CICECO was held in Aveiro (23rd – 27th May) purposed to join together specialists from the different areas of materials science, such as materials chemists and processing engineers, diffraction and spectroscopy scientists, and structural computational, that may contribute to the development of a common language for a SMARTER approach to structure solving, using geometrical, diffraction modeling and NMR crystallography.

The event counted with over 120 scientists from more than twelve countries to review and discuss ideas in the field (http://smarter.web.ua.pt/).

SMARTER workshop on CICECO, Universidade de Aveiro.

June

PTNMR Sponsored Conference – 3rd EU/CCPN Conference

The European CCPN Conference under the title: Solids, Solutions and Samples held in Oeiras, was jointly organised by the NMR group at ITQB and the IGC (http://www.ccpn.ac.uk/meetings/pastmeetings/2011euccpn). During the 3-day conference it was presented current best practices for different aspects of macromolecular NMR,

from sample preparation to liquids and solids NMR. The conference was accompanied by a satellite course given by the CCPNMR team from the University of Cambridge, sponsored by the BBSRC, UK. This course held at IGC, have demonstrated and tutored national NMR users for the advantage of using CCPNMR Analysis software in their daily basis, as currently being widespread in the international NMR community.

Poster layout of the European CCPN Conference held in Oeiras 28th – 30th September.

July

PTNMR Sponsored Course - V Hands-on Course: From Proteomics to Proteins

Biomolecular NMR lecture module in the V Hands on Course between 3 to 16 July. The aim was to provide basic knowledge about fundamentals on NMR spectroscopy for biomolecular sciences.

Eurico J. Cabrita received the Vicente de Seabra Medal from the Portuguese Chemical Society

The Portuguese National NMR Network (PTNMR) Coordinator, Dr. Eurico J. Cabrita has been awarded the Vicente de Seabra Medal 2010 of the Portuguese Chemical Society (SPQ). He received the medal for his contribution in the NMR field in Portugal. He was one of the foremost important young researchers to contribute for the development and establishment of the NMR field in Portugal and made decisive contributions to the foundation of the national NMR network, what is know today as the PTNMR. The award ceremony of the medal took place on July 3- 6 during the annual meeting of the Portuguese Chemical Society in Braga.

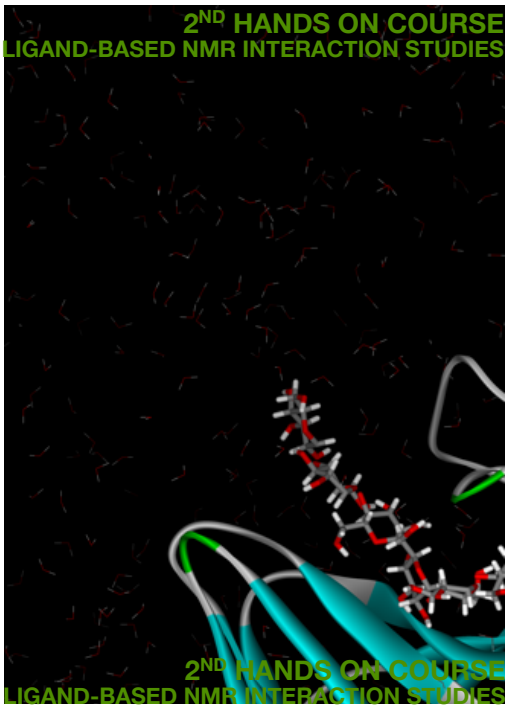
INSERT EURICO PHOTO

Dr. Eurico J. Cabrita at the award ceremony with the president of SPQ at the annual meeting of the Portuguese Chemical Society.

September

PTNMR Course - 2nd Hands on Course on Ligand based NMR interaction studies

This course organised by the NMR group of REQUIMTE/ FCT-UNL between 12th and 15th September at the Chemistry Department, FCT, Monte da Caparica, was focused on the fundamentals of diffusion and NOE based experiments. The course was intended for PhD students and NMR technicians who already have a thorough knowledge of NMR spectroscopy, and has counted with participants from academia and industry. The attendees seemed to appreciate the fact that all sessions left ample time for discussions and questions. The active participation of the attendees in the discussions during the lectures was very stimulating.



Poster of the Course Caparica 12th – 15th September.

PTNMR Seminar – Prof.John C. Lindon – ICL,London

Prof. John C. Lindon from the Department of Biomolecular Medicine, Imperial College London has given a talk under the title: Bringing molecules into medicine using NMR and mass spectrometry based metabonomics. The talk was given in Universidade de Aveiro, 21st September and it was intended to promote discussion and exchange of ideas. This talks have a higher pedagogical content where Diploma, MSc. and PhD students are encourage to participate asking questions.

October

PTNMR Seminar – Dr. Flemming Hansen – ICL, London

Dr. Dennis Hansen from ISMB, University College London was invited by the REQUIMTE/FCT-UNL pole to give a talk on Structure and Dynamics of Excited and Invisible Protein States: Application to chromatin remodelling and protein folding. He has been developing NMR methodologies to study protein dynamics and to characterise thermally excited and low populated states of proteins.

November

ENERMATaa

A short-introductory course lectured by Joao Rocha (CICECO-Univ. de Aveiro) was made in the ENERMATaa Training course-Nanomaterials and Hybrid Materials, held in Aveiro between 24th and 25th November.

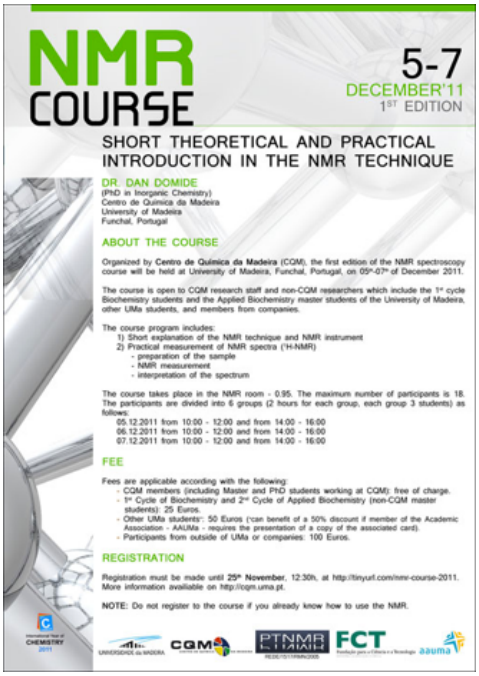
PTNMR Course - School on Modern Methods of Structure Elucidation

A NMR course was lectured in IST-UTL Lisbon dedicated to different NMR and EPR spectroscopic techniques (http://cqe.ist.utl.pt/events/mmse2011/). The training course on modern spectroscopic analytical techniques was intended for bachelors, masters, PhD and PostDoc from universities across the country. The school included theoretical sessions provided by recognised specialists in the field, practical sessions and demonstrations on the equipment supported by the National NMR Network. This event has provided the possibility for students and researchers to get hands-on training with the equipment.

December

PTNMR Course - Short theoretical and practical introduction in the NMR techniques

This first edition of the course organised by the NMR group from the CQM - Universidade da Madeira covered some basics in the NMR spectroscopy. The aim of the course was to tutor and demonstrate the importance of NMR spectroscopy in the CQM research.



Poster layout of the *Short theoretical and practical introduction in the NMR technique* (5th-7th December 2011) held in Madeira Chemistry Research Center.

2012

February

2nd PTNMR National Meeting / Bruker Users Meeting – FCT/UNL, Caparica

Under the topic *NMR in Portugal an overview* this scientific meeting highlighted the current research done in Portugal in the last year. The meeting that gathered researchers from all PTNMR affiliated centers provided an excellent networking opportunity for students and researchers to present their research topics and to share ideas to relevant current project needs. The meeting provided a venue for presentation of a broad range of NMR applications across the country and a forum for discussion of methods driving further development of the NMR field in Portugal.

This event was preceded by the Bruker users meeting presenting the latest hardware- and software developments at Bruker. The meeting had 92 participants with a scientific programme that included 10 oral communications and 51 poster communications.

Library Auditorium 3rd February 2012

http://eventos.fct.unl.pt/jornadasrmn/

PTNMR Course - NMR Course from Theory to Practice

Following the compromise established by the PTNMR network of mentoring and spreading the knowledge of NMR in Portugal, it was held in Centro de Investigacao em Ciencias da Saude, Faculdade de Ciências da Saude, Universidade da Beira Interior, Covilha, the NMR course: from theory to practice. This course co-organized by the REQUIMTE/DQ/FCT-UNL NMR unit team between 13th to 17th February 2012 (www.ubi.pt/Ficheiros/Noticias/FCS/Curso_Covilha_final.pdf) covered basic theory of NMR spectroscopy combined with practical aspects of NMR acquisition and processing. Standard 1D and 2D NMR techniques were employed by the students for structural analysis. During the course the students were able to interact with the spectrometer and analyze their own data. This course follows-up previous editions in 2010 and was focused mainly for PhD, and Master students from Portuguese academia.

Poster layout of the *Hands on Course, NMR - From theory to Practice* (13th-17th February 2012) held in Health Sciences Research Centre, Covilha.

March

PTNMR Seminar – Prof. Kevin Brindle – University of Cambridge

The PTNMR seminars are intended to encourage scientific discussion and to promote collaboration and knowledge transfer by encouraging interaction within the portuguese research scientific community. Following that, Prof. Kevin Brindle a recognised specialist in the MRI field was invited to give a seminar on the Center for Neuroscience and Cell Biology (CNC), Universidade de Coimbra. The title of his talk was: “Hiperpolarized 13C-labeled substrates for metabolic MR imaging of pathologies”, 29th March 2012. This was a great opportunity for researchers and students to meet the scientist and discuss the latest developments on the MRI field.

April

Reach out Activities – ExpoFCT

This open day activity is promoted by the Faculdade de Ciências e Tecnologia, Caparica, as an outreach activity towards the population in general and the students of secondary schools. The researchers and staff of the NMR lab were associated with this initiative and organized guided tours to the NMR laboratories. During the tours general explanations were given about the research work being supported and conducted in the lab.

May

PTNMR Seminar – Prof. Stefan Berger –Leipzig University

Following up the very active programme of seminars and lectures, given by external, invited speakers, the NMR unit at REQUIMTE/DQ/FCT-UNL has invited Prof. Stefan Berger for a lecture on NMR Hyperpolarization by the Haupt effect (25th May 2012) . Prof. Stefan Berger is a well-know NMR spectroscopist and author of several NMR books including 100/150/200 and More NMR Experiments, 13C NMR Spectroscopy, and Classics in Spectroscopy. Prof. S. Berger received the Fonds der Chemischen Industrie's Literature Prize in 2009, an award that recognizes authors of outstanding chemistry books.

http://ptnmr.dq.ua.pt/index.php/activities/seminars/168-ptnmr-seminars-fctunl

June

PTNMR Seminar – Prof. Malcolm Levitt –University of Southampton

Prof. Malcolm Levitt from the University of Southampton was invited by the Portuguese NMR network to give a 1h30 lecture about his most recent research work under the topic of Singlet Nuclear Magnetic Resonance. The audience was composed of members of the PTNMR network from the Aveiro and Lisbon NMR centers, as well as several other researchers from the University of Aveiro. In the following day, June 20th, 2012, Prof. Malcolm Levitt gave a 3h workshop on SpinDynamica, a set of packages for Mathematica intended for NMR calculation and simulation, programmed by his research group. This session was mainly directed to solid-state NMR users and several examples were presented regarding concrete solid-state NMR problems.

http://ptnmr.dq.ua.pt/index.php/activities/seminars/174-ptnmr-seminar-aveiro

PTNMR Course –NMR Basics: Theory, Processing and Applications

A five days course entitled "NMR Basics: Theory, Processing and Applications" was held in Coimbra from June 11th to June 15th 2012. The course, organized by LabRMN-CNC and L-RMN-CQC, took place in the Chemistry Department of FCTUC and CNC, University of Coimbra, and was oriented towards beginners discovering the NMR technique and for those who want to use it as a tool for their research work. The course covered theoretical

lectures and "hands-on" sessions at NMR labs (NMR spectrometers: Varian Unity 500 MHz and VNMRS 600 MHz, Bruker Avance III 400 MHz) and in computer room for data processing and spectral analysis. The program covered standard and advanced 1D/2D/3D experiments, multinuclear NMR towards structural analysis and dynamics of small and large molecules. It also highlighted to the use of the NMR technique as an important tool to be used in the study of small organic molecules, proteins, biological systems and in clinical applications (NMR of cells and organs, metabonomics, MRS ex vivo and in vivo, MRI).

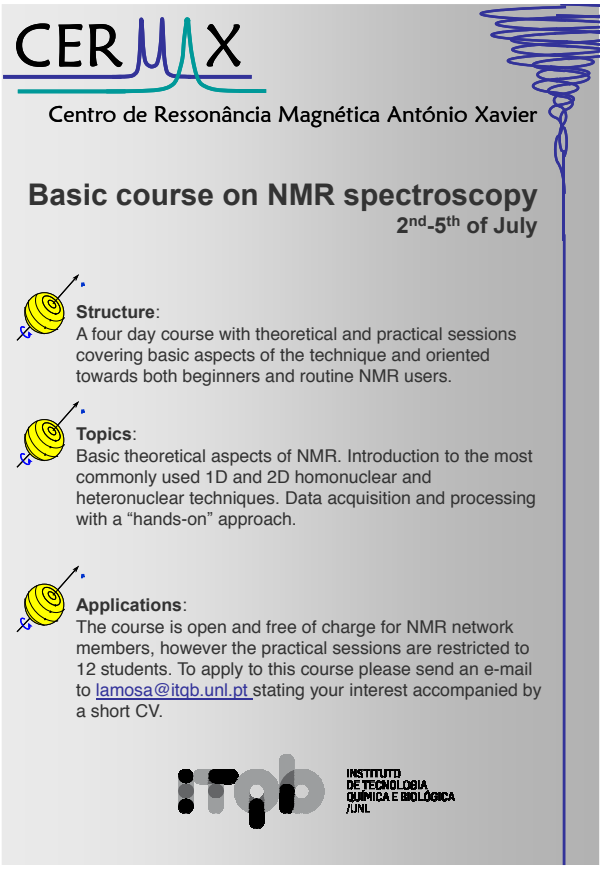
July

PTNMR Sponsored Course - V Hands-on Course: From Proteomics to Proteins

Biomolecular NMR lecture module in the V Hands on Course between 3rd to 16th July. The aim was to provide basic knowledge about fundamentals on NMR spectroscopy for biomolecular sciences.

PTNMR Course – 5th CERMAX practical course on basic NMR

A four-day course with theoretical and practical sessions covering basics aspects of the technique and oriented towards both beginners and routine NMR users. The course, organized by CERMAX/ITQB, took place at ITQB between 2nd and 5th of July. The topics covered included basic theoretical aspects of NMR, introduction to the most commonly used 1D and 2D homonuclear and heteronuclear techniques, data acquisition and processing with a “hands-on” approach. This course was part of the PhD training course at ITQB.



Poster layout of the 5th CERMAX practical NMR course, held at ITQB-UNL, Oeiras.

http://www.itqb.unl.pt/events/courses/5th-cermax-practical-course-on-basic-nmr

September

PTNMR Conference – IV Ibero-American NMR meeting – VI GERMN Bienal Meeting – III Iberian NMR meeting

One of the main NMR events in 2012 in Portugal has jointed the Luso-Spanish-Brazilian NMR societies in a large event in Aveiro. The IV Ibero-American NMR Meeting organized by the Portuguese NMR Group of the Portuguese Chemical Society aimed to strength the link between the Spanish and South American NMR societies, to foster the exchange and sharing of scientific ideas on all aspects of NMR between colleagues of both countries. The event was co-organized by several PTNMR members (Chairman: Luís Mafra and Eurico Cabrita) and was

attended by 200 specialists in NMR arising from Portugal, Spain, France, Germany, Italy, Belgium, Check Republic, Netherlands, Sweden, Canada, UK and USA. The scientific programme consisted of 6 plenary talks, 4 invited talks, 9 key-note talks, 25 talks, and 124 posters. This conference invited a broad scientific community to present their results from across different fields of NMR spectroscopy. A peer-reviewed selection of poster applications and invitation for oral presentation were selected for the conference.

The conference was precede with a one-day course in metabonomics and solid-state NMR, organised by Dr. Luis Mafra, Dr. Ana Gil, Dr. Brian Goodfellow and Dr. Iola Duarte, all members of the CICECO research Lab (Aveiro).

Group photo of the IV Ibero-American NMR meeting – VI GERMN Bienal Meeting – III Iberian NMR meeting, held in Aveiro (25th and 28th September 2012).

http://www.spq.pt/eventos/iberoanmr2012/

SMARTER 3 Conference - Diffraction, Modeling, Magnetic Resonance

This international conference, SMARTER that stands for Structure elucidation by coMbining mAgnetic Resonance, compuTation modEling and diffRactions aims to bring together specialists from the different areas of material sciences, such as chemists, processing engineers, diffractionists, spectroscopists, and computational structuralists that contribute to the development of a common language for SMARTER Crystallography, i.e. for solving structures by using geometrical crystallography, diffraction, modeling and NMR cristallographies. This prestigious conference was co-organised by a PTNMR member, Prof. Joao Rocha (CICECO), and was held at the University of Versailles Saint-Quentin-en-Yvelines, France.

November

PTNMR Courses - School on Modern Methods of Structure Elucidation

As succeed in each year, the IST/UTL NMR affiliated center organized the *School on Modern Methods of Structure Elucidation* (MMSE-2012), covering a wide range of spectroscopic techniques for structural elucidation. The school is addressed to young scientists (post graduate students, PhD students and post-doctoral fellows) and is focused on theoretical and experimental aspects of solution and solid-state NMR, X-ray diffraction, EPR and mass spectrometry. At the end of the school, students should be able to solve structural problems recurring to the different techniques learnt.

Program flyer of the School on Modern Methods of Structure Elucidation (MMSE-2012) held on IST/UTL - Lisbon between 12th and 16th November 2012.

http://cqe.ist.utl.pt/events/mmse/next.php

December

PTNMR Course – NMR of small molecules in aligned media

The workshop organised by the NMR Unit at the Chemistry Department of Faculdade de Ciências e Tecnologia - Universidade Nova de Lisboa (REQUIMTE/DQ/FCT-UNL), Caparica (Portugal) was intended to provide theoretical and practical training in important aspects of aligned media for structural elucidation of small molecules and the measurement of residual dipolar couplings (RDC). The emphasis of the training was on setting up experiments on the spectrometer (optimizing parameters, pulse programs), preparing samples as well as processing and analysing NMR data. This course has counted with the participation of Dr. Armando N. Vazquez from Universidade de Vigo (Spain) as a lecturer.

http://eventos.fct.unl.pt/alignmr/

Poster layout of the course held in Madeira Chemistry Research Center.

PTNMR Course – Short theoretical and practical introduction in the NMR technique

The Madeira Chemistry Research Center organised an introductory course on NMR spectroscopy for undergraduate, Master and PhD students associated to the Madeira University. This introductory course was intended for students at undergraduate and post-graduate level who intend to make use of NMR in their research. The course was descriptive rather than mathematical. The focus of the course was on the technique and in the interpretation of NMR spectra. The course was practical with hands-on the machine.

Research Highlights

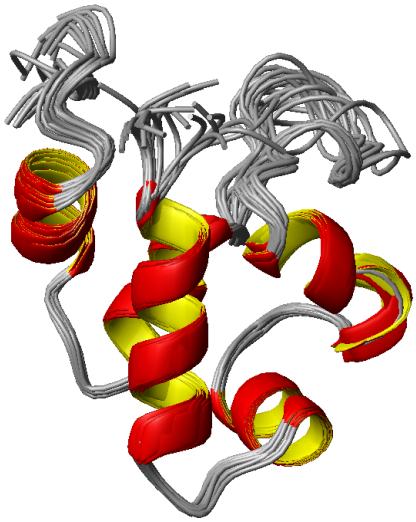
Structural Biology

NMR investigation of the *Bacillus subtilis* morphogenic factor RodZ

Ana Catarina Pereira, Ana Almeida, Teresa Costa, Adriano O. Henriques, Manolis Matzapetakis

Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Av. da República – EAN, 2780-157 Oeiras, Portugal.

RodZ is a multi-domain protein, involved in morphogenesis and is widely conserved in both gram negative and gram positive bacteria. Its N-terminal domain (RodZ-N), located in the cytoplasm, has been shown to interact with Actin by functional and crystallographic studies in *Thermotoga maritima* [1].



The *Bacillus subtilis* RodZ-N, has low homology (<30%) compared to its *Thermotoga maritima* homologue. Recent data on *Bacillus subtilis* suggest a potentially different cellular function for it with the possibility of it being involved in DNA organization. In order to evaluate if the differences in behavior between the *Bacillus subtilis* and the *Thermotoga maritima* RodZ-N are based on structural differences, we set out to structurally characterize it by NMR.

We have collected and analyzed triple resonance NMR spectra for the complete resonance assignment of RodZ-N. 78% of the resonances have been identified, however, no amides in the region of 47-54 could be observed in the 15N HSQC spectrum. The resulting protein structure was determined to have a helix-turn-helix motif with high similarity to the previously characterized structure with the exception of an extended unstructured region which may be related to its proposed new functionality.

Acknowledgements

We acknowledge CERMAX at ITQB and Rede Nacional de RMN for access to the facilities, supported with funds from FCT, Projecto de Re-Equipamento Científico (REDE/1517/RMN/2005).

References

[1] van den Ent F, Johnson CM, Persons L, de Boer P & Löwe J (2010) Bacterial actin MreB assembles in complex with cell shape protein RodZ. EMBO J. 29, 1081-90.

How bacteria do their math; bacteria can count their numbers, but they can also, potentially, be fooled

João C. Marques[1], Pedro Lamosa[1], Caitlin Russell[2], Rita Ventura[1], Christopher Maycock[1], Martin F. Semmelhack[3], Stephen T. Miller[2] and Karina B. Xavier[1]

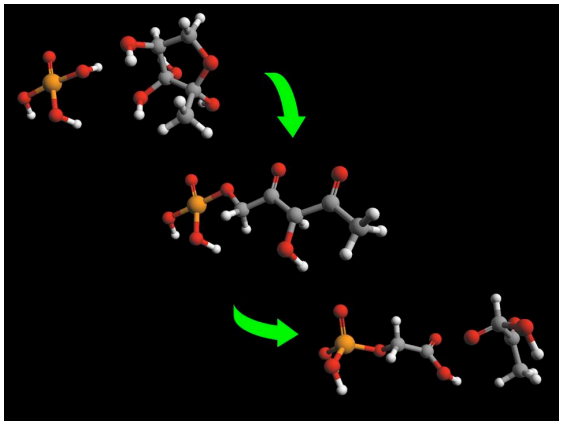
[1]Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Av. da República – EAN, 2780-157 Oeiras, Portugal. [2]Department of Chemistry and Biochemistry, Swarthmore College, Swarthmore, Pennsylvania 19081, [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544

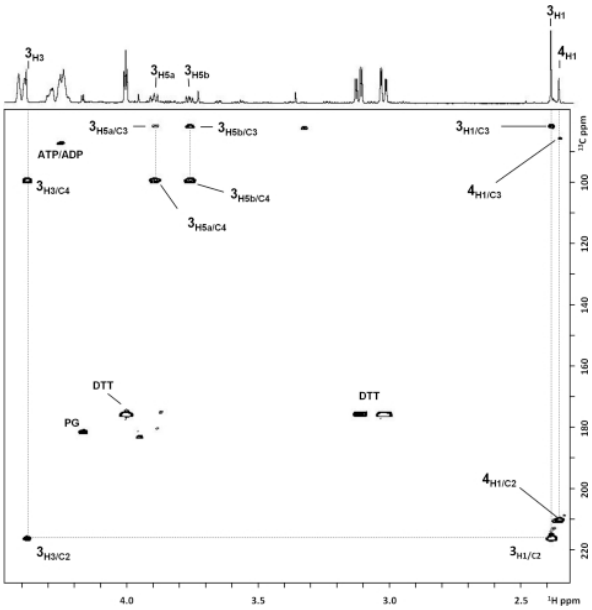
Many bacteria regulate gene expression as a function of the density of the population in a process called quorum sensing, which enables these organisms to coordinate important bacterial behaviours such as biofilm formation and the production of virulence factors. Quorum sensing is mediated by signal molecules called autoinducers. One autoinducer (Autoinducer-2, AI-2) is produced by many species of bacteria and can facilitate inter-species cell-cell signalling.

The way in which the production of this molecule is regulated has been known for some time (it is a virtuous circle in which the concentration of AI-2 stimulates its own production), but its degradation was still not clear. In fact, certain bacteria (like *E. coli* and *Salmonella typhimurium*) are able to process the signal, thus, quenching inter-species communication and fooling other members of the bacterial community as to their real numbers.

In this work, using *in vivo* and *in vitro* NMR, we have shown that the first step in the catabolic reaction in *E. coli* is the isomerisation of the phosphorylated signal molecule into an unstable intermediate (3,4,4-trihydroxy-2-pentanona-5-phosphate). Using two dimensional ^{13}C-^{1}H and ^{31}P-^{1}H spectroscopy it was possible to fully characterise the metabolic degradation pathway and unveil the chemical structure of the intermediates. The X-ray structure of this new isomerase allowed determining its active site, which was confirmed by site-directed mutagenesis.

This discovery may pave the way into new methodologies of quenching the interspecies signalling mechanisms, which can be of great utility in the development of therapies to control bacterial behaviour.





Acknowledgments

We thank Ana R. Neves and Teresa Catarino for precious help in optimizing the NMR conditions and preparing the anaerobic samples, respectively. The NMR spectrometers are part of The National NMR Network (REDE/1517/RMN/2005), supported by "Programa Operacional Ciência e Inovação (POCTI) 2010" and Fundação para a Ciência e Tecnologia. We acknowledge National BioResource Project (Japan):E. coli for providing strain JCM62

References

Marques JC, Lamosa P, Russell C, Ventura R, Maycock C, Semmelhack MF, Miller ST & Xavier KB. (2011) Processing the interspecies quorum-sensing signal autoinducer-2 (AI-2): characterization of phospho-(S)-4,5-dihydroxy-2,3-pentanedione isomerization by LsrG protein *J Biol Chem.* 286, 18331-43.

Paramagnetic probes to study transient protein interactions and protein assisted cluster biosynthesis studied by NMR

Almeida RM, Moura I, Moura JJG, Pauleta SR

REQUIMTE-CQFB, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal

NMR methods (^{1}H and 2D NMR spectra and paramagnetic probes) have been used to characterize transient protein complexes involved in the denitrification pathway,[1,2] and detoxification of reactive oxygen species, such as superoxide anion and hydrogen peroxide (Almeida *et al*., unpublished). In *Desulfovibrio gigas*, a strict anaerobic bacterium, superoxide reductase (SOR) is responsible for the reduction of superoxide anion to hydrogen peroxide, which is generated when the bacteria is transiently exposed to oxygen. The electron transfer complexes between SOR and its electron donors, rubredoxin and desulforedoxin, were characterized using NMR spectroscopy to determine the stoichiometry and model structure of these complexes. The methodology used in these studies included the use of non-covalently bound paramagnetic probes and NMR competition binding studies Almeida *et al*., unpublished). These probes have also been used in the characterization of a model system the transient complex between rubredoxin and cytochrome c_3 (Figure 1).[3,4]

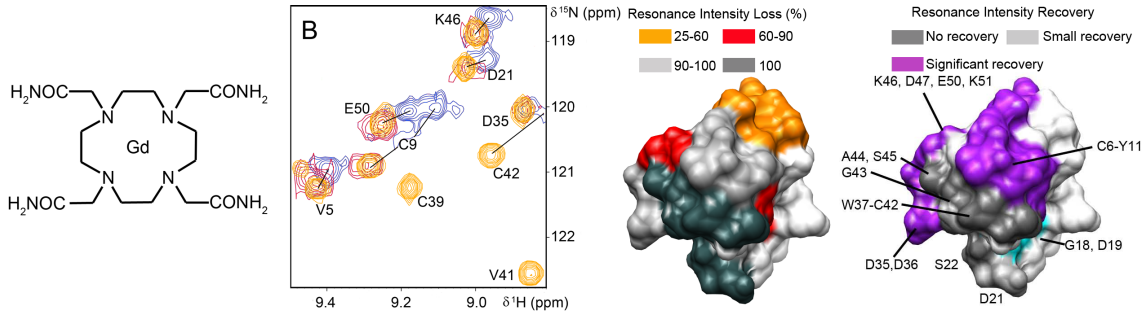


Figure 1 – A) Gd-DOTAM – a cyclen ring with four acetamide substituents bound to the ring nitrogens. B) ^{1}H-^{15}N HSQC of Zn-rubredoxin (Orange), Rubredoxin:Gd-DOTAM 1:1 (Red), Rubredoxin:Gd-DOTAM:cytochrome c3 1:2:2 (blue). C) Left: Surface mapping of resonance intensity loss of rubredoxin upon addition of Gd-DOTAM 1:1; Right: Resonance intensity recovery upon addition of cytochrome c_3.

Hydrogen peroxide is formed under hypoxic conditions as a result of the restriction in the flow of electrons in the electron transport chain. Thus, many proteobacteria express in their periplasm a cytochrome *c* peroxidase under these conditions to reduce hydrogen peroxide to water. The transient complexes formed between this enzyme and its electron donors have been characterized using NMR, kinetics and isothermal titration calorimetry (Pauleta *et al*., unpublished).
The ORange Protein (ORP) from *Desulfovibrio gigas* is an orange coloured 11.8 kDa protein that contains a mixed-metal sulphide cluster, of the type $[S_2MoS_2CuS_2MoS_2]^{3-}$, non-covalently bound to the polypeptide chain.[5] A blast search revealed that this protein has sequence homology of around 30 to 50 % with conserved proteins from eubacteria and hyperthermophilic archaea with unknown function. They all contain a conserved domain common to the nitrogenase accessory factor (NifB C-terminal domain, NifX and NafY).
The solution NMR structure and dynamic characterization of this protein in the apo- and reconstituted form enabled the identification of the residues involved in cluster binding.[5] The NMR results indicate that the mechanism of cluster biosynthesis involves a protein assisted mechanism (Pauleta *et al*., unpublished) (Figure 2).

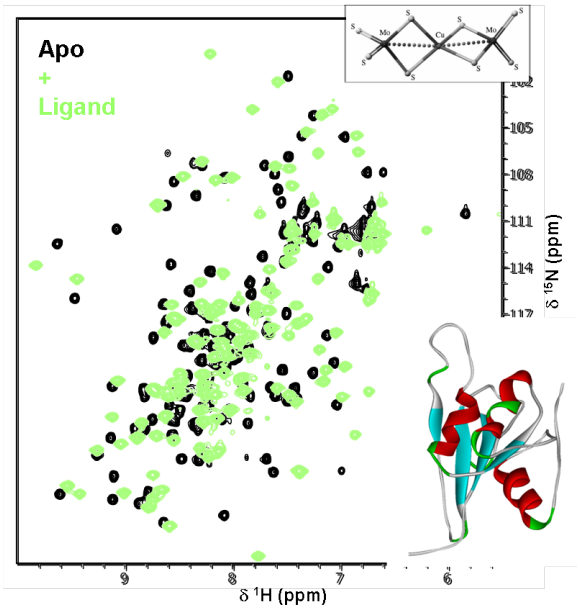


Figure 2 – ^{1}H-^{15}N HSQC of the apo-ORP (black) and reconstituted ORP (green). In the bottom it is shown the structure of the reconstituted ORP determined by NMR.

This protein is part of a conserved operon that has been shown to be associated with the anaerobic mode of life.[6] Moreover these results give insights into the metal binding mode of chaperons involved in the synthesis of the nitrogenase metal cofactor.

Funding

We thank Fundação para a Ciência e Tecnologia for financial support (PPCDT/QUI/57741/2004, PTDC/BIA-PRO/109796/2009, PTDC/BIA-PRO/098882/2008, PTDC/QUI-BIQ/098071/2008), and PhD and post-doctoral grant (RMA). The NMR spectrometers (600 MHz and 800 MHz) are part of the National NMR Network (RNRMN) and are funded by Fundação para a Ciência e a Tecnologia (FCT).

References

[1] Dell'Acqua S, Pauleta SR, Monzani E, Pereira AS, Casella L, Moura JJG, Moura I, "Electron transfer complex between nitrous oxide reductase and cytochrome c_{552} from Pseudomonas nautica: kinetic, nuclear magnetic resonance, and docking studies", *Biochemistry* **2008**, 47, 10852-10862
[2] Dell'Acqua S, Moura I, Moura JJG, Pauleta SR, "The electron transfer complex between nitrous oxide reductase and its electron donors", *Journal of Biological Inorganic Chemistry* **2011**, 16, 1241-1254
[3] Almeida RM, Pauleta SR, Moura I, Moura JJG, "Rubredoxin as a paramagnetic relaxation-inducing probe", Journal of Inorganic *Biochemistry* **2009**, 103, 1245-1253
[4] Almeida RM, Geraldes CFGC, Pauleta SR, Moura JJG, "Gd(III) chelates as NMR probes of protein-protein interactions. Case study: rubredoxin and cytochrome c_3", *Inorganic Chemistry* **2011**, 50, 10600-10607
[5] Pauleta SR, Duarte AG, Carepo MS, Pereira AS, Tavares P, Moura I, Moura JJG, "NMR assignment of the apo-form of a Desulfovibrio gigas protein containing a novel Mo-Cu cluster", *Biomolecular NMR Assignments* **2007**, 1, 81-83
[6] Fiévet A, My L, Cascales E, Ansaldi M, Pauleta SR, Moura I, Dermoun Z, Bernard CS, Dolla A, Aubert C, "The anaerobe-specific orange protein complex of Desulfovibrio vulgaris Hildenborough is encoded by two divergent operons coregulated by σ54 and a cognate transcriptional regulator" *Journal of Bacteriology* **2011**, 193, 3207-3219

NMR insights into the mechanism of molecular selectivity and recognition by carbohydrate-binding modules from *Clostridium thermocellum*

Viegas A., Sardinha J., Carvalho A.L., Macedo A., Cabrita, E. J.

REQUIMTE/CQFB, Department of Chemistry, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal.

The direct conversion of plant cell wall polysaccharides into soluble sugars is one of the most important reactions on earth, and is performed by certain microorganisms such as Clostridium thermocellum. These organisms produce extracellular multi-subunit complexes, called cellulosomes that include a consortium of enzymes, which contain non-catalytic Carbohydrate-Binding Modules (CBM), that increase the activity of the catalytic module. The catalytic mechanisms of the enzymes present in the cellulosome are well understood, but the function and behaviour of the CBMs have not yet been fully elucidated. In order to deeply understand the molecular interactions that define the ligand specificity in cellulosomal CBMs and the mechanism by which they recognize and select their substrates, we combine NMR spectroscopy, X-ray crystallography and molecular modelling to identify the molecular determinants of ligand specificity of several type B CBMs from C. thermocellum.[1,2] The strategy includes: (i) the identification of the ligand atoms responsible for binding to the protein through STD-NMR experiments,[1] (ii) protein structure determination and identification of the protein residues responsible for ligand recognition by NMR titrations with selected oligosaccharides[2,3], (iii) atomistic rationalization of the determinants of ligand specificity based on the combination of NMR data with molecular modelling (docking and molecular dynamics)[2,3]. Our results allow an understanding, at the molecular level, of the interactions that define the ligand specificity in cellulosomal CBMs and the mechanism by which they recognize and select their substrates.

We have determined the NMR solution structure of *Ct*CBM11 at 25 and 50 ºC and derived information on the residues of the protein involved in ligand recognition and on the influence of the length of the saccharide chain on binding (figure 1).[2,3]

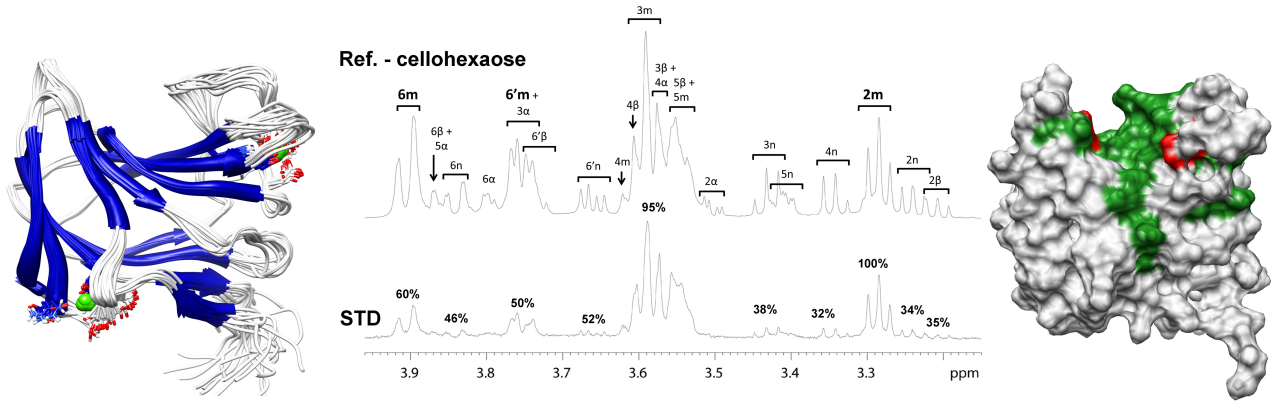


Figure 1 - A) NMR solution structure of CtCBM11 at 50 ºC. B) Interaction studies between *Ct*CBM11 and cellohexaose B1) ligand based experiments using STD-NMR; B2) Identification of the binding cleft of *Ct*CBM11 based on NMR titrations.

We obtained models of the *Ct*CBM11/cellohexaose and *Ct*CBM11/cellotetraose complexes by docking in accordance with the NMR experimental data. Specific ligand/protein CH-π and Van der Waals interactions were found to be determinant for the stability of the complexes and for defining specificity (figure 2). We have identified CH-π interactions with Tyr53 and Tyr129 that stabilize the conformation of the ligands in the binding cleft.

A reduction of the size of the oligosaccharide leads to the weakening of the CH-π interaction with Tyr53, which seems to be responsible for the difference in affinity observed with cellotetraose when compared to cellohexaose. The contacts that CtCBM11 makes with the OH groups attached to carbons 2 and 6 from the central glucose units allied to the rigid conformation of the cleft are determinant to the specificity of the protein. Only ligands with a methylene group at C5, with the OH group at C2 in an equatorial position and displaying the typical twisted conformation of β-1,4-linked glucans can bind to this protein. Analysis of the in silico bound carbohydrate conformations reveals that CtCBM11 recognizes conformations that are energy minimum in solution, consistent with the observations for other type B CBMs. These observations combined with thermodynamic data, extracted from protein relaxation studies, supported by previous ITC experiments, indicate that CtCBM11/ligand recognition is consistent with a rigid protein backbone that selects a defined oligosaccharide conformation that in this case is coincident with the minimum energy conformation existent in solution. We postulate that the loss in entropy associated with ligand binding (due to conformational space restrictions) may be responsible for the overall negative binding entropy.[3]

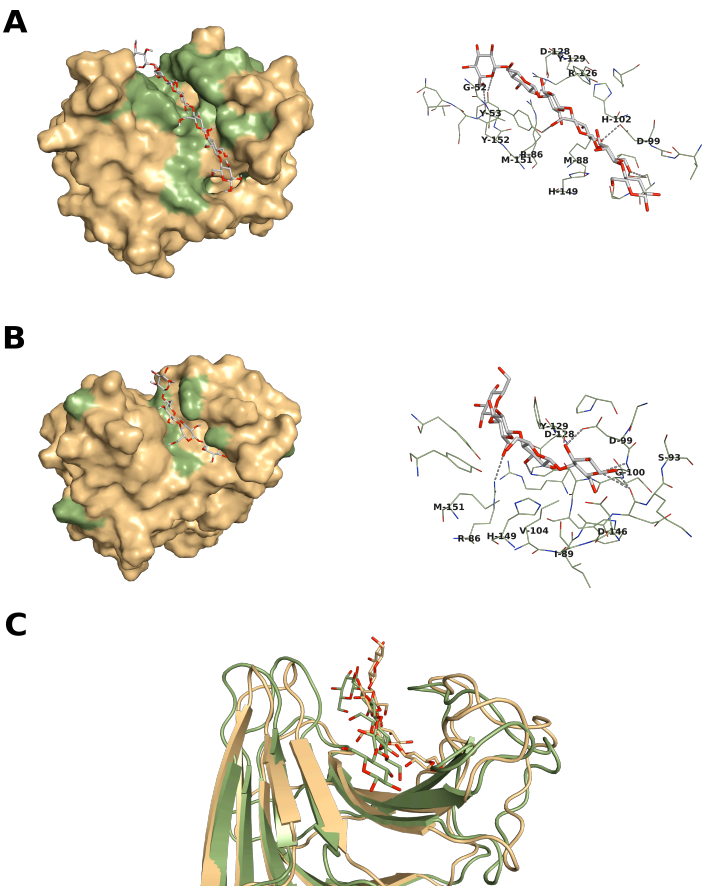


Figure 2 - Molecular Dynamics models of CtCBM11 with cellohexaose (A) and cellotetraose (B) at 25 ºC and superposition of both strutures (C). Right - highlight of the cleft of the complex denoting some of the polar contacts occurring between ligand and receptor (gray dashed lines).

Funding

This work was supported by Fundação para a Ciência e a Tecnologia (FCT) through projects [PTDC/QUI-QUI/098892/2008] and [PTDC/QUI-BIQ/100359/2008] and grants [SFRH/BD/35992/2007] and [SFRH/BD/30239/2006]. The NMR spectrometers are part of the Portuguese National NMR Network (RNRMN) supported with funds from FCT.

References

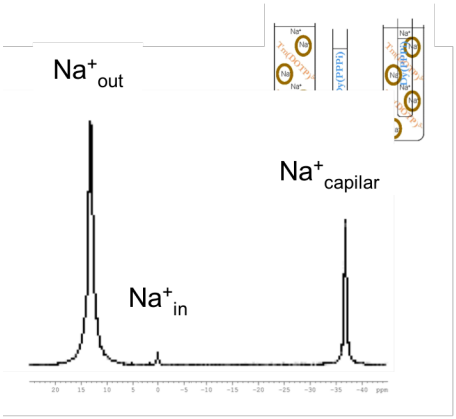
[1] Viegas A, Bras NF, Cerqueira NMFSA, Fernandes PA, Prates JAM, Fontes CMGA, Bruix M, Romao MJ, Carvalho AL, Ramos MJ, Macedo AL, Cabrita, EJ "Molecular determinants of ligand specificity in family 11 carbohydrate binding modules - an NMR, X-ray crystallography and computational chemistry approach" *FEBS J.*, **2008**, 275, 2524-2535.
[2] Viegas A "Molecular Determinants of Ligand Specificity in Carbohydrate-Binding Modules: an NMR and X-ray crystallography integrated study", PhD Dissertation, Universidade Nova de Lisboa, **2012**.
[3] Viegas A, Sardinha J, Freire F, Duarte DF, Carvalho AL, Fontes CMGA, Romão MJ, Macedo AL, Cabrita EJ, "Solution Structure, Dynamics and Binding Studies of a Family 11 Carbohydrate-Binding Module from Clostridium thermocellum (CtCBM11)", *Biochemical Journal*, **2013**, in press.

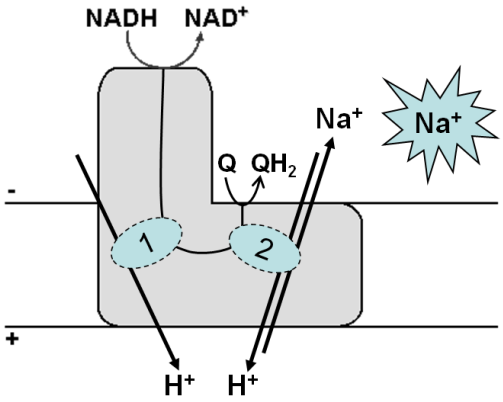
New Insight Into the Respiratory Complex I Using ^{23}Na-NMR Spectroscopy

Ana P. Batista, Andreia S. Fernandes, Bruno C. Marreiros, Ricardo O. Louro and Manuela M. Pereira

Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Av. da República – EAN, 2780-157 Oeiras, Portugal.

The research on complex I has gained recently a new enthusiasm, especially after the resolution of the crystallographic structures of bacterial and mitochondrial complexes. Most attention is now dedicated to the investigation of the energy coupling mechanism(s). The proton has been identified as the coupling ion, although in the case of some bacterial complexes I sodium has been proposed to have that role.
We have addressed the relation of complex I with sodium by developing an innovative methodology using 23Na-NMR spectroscopy, with the advantage of allowing a direct observation of the sodium nuclei via its own resonance frequency. We used membrane vesicles and sodium ions at the different compartments could be monitored and calibrated using shift reagents.
We have shown that, in fact, some bacterial complexes I are capable of proton and sodium translocation, but to opposite directions, being the proton the coupling ion. A model for the functional mechanism of complex I was then proposed, suggesting the presence of two different energy coupling sites, both operating by indirect coupling mechanisms. One coupling site may work as a proton pump and the other as a Na^+/H^+ antiporter.





Acknowledgements

We acknowledge CERMAX at ITQB and Rede Nacional de RMN for access to the facilities, supported with funds from FCT, Projecto de Re-Equipamento Científico (REDE/1517/RMN/2005). A. S. Fernandes was recipient of a grant from Fundação para a Ciência e a Tecnologia (SFRH/BPD/34493/2006). A. P. Batista is recipient of a grant from Fundação para a Ciência e a Tecnologia (SFRH/BD/25288/2005). This project was funded by Fundação para a Ciência e a Tecnologia (POCI/BIA-PRO/58374/2004 and POCI/QUI-BIQ/100302/2008 to M.P., FCT-REEQ/336/BIO/2005 to ITQB) and by the Parkinson Schweiz (to J. S.).

References

Batista AP, Fernandes AS, Louro RO, Steuber J, & Pereira MM. (2010) Energy conservation by Rhodothermus marinus respiratory complex I. Biochim Biophys Acta. 1797, 509-15

NMR AS A TOOL FOR THE IMPROVEMENT OF BACTERIAL BIOREMEDIATION AND ELECTRICITY HARVESTING SKILLS: STRUCTURAL AND FUNCTIONAL STUDIES

Leonor Morgado, Ana P. Fernandes, Joana M. Dantas, Marta A. Silva, Carlos A. Salgueiro

Requimte-CQFB, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal.

Extracellular electron transfer in *Geobacter* species is one of the physiological hallmarks of these bacteria.[1] *Geobacter* species can precipitate toxic and/or radioactive metals such as uranium by using these metals as a terminal acceptor, reducing the oxidized, soluble form of the metals to insoluble reduced forms. They can also couple the oxidation of organic compounds coupled to electron transfer to electrodes offering the possibility of converting organic waste materials and renewable biomass to electricity. These properties could conceivably be enhanced for practical applications by genetically engineering bacterial strains or by functional optimization of the respiratory electron transfer chains. One of the most striking features of *Geobacter* species is the abundant and the large diversity of *c*-type cytochromes encoded in its genome, most of which are multihemic.[2-3] Genetic studies with *G. sulfurreducens* (*Gs*) strains with the genes encoding multiheme cytochromes deleted showed the involvement of these proteins in the extracellular electron transfer pathways.[1]

The characterization of the functional mechanism of multiheme proteins is particularly complex due to the coexistence of several microstates in solution, connecting the fully reduced and oxidized states.[4] To obtain information of each microstate it is necessary to monitor the stepwise oxidation of each individual heme, which for the particular case of heme groups displaying identical optical properties can only be obtained by NMR spectroscopy.

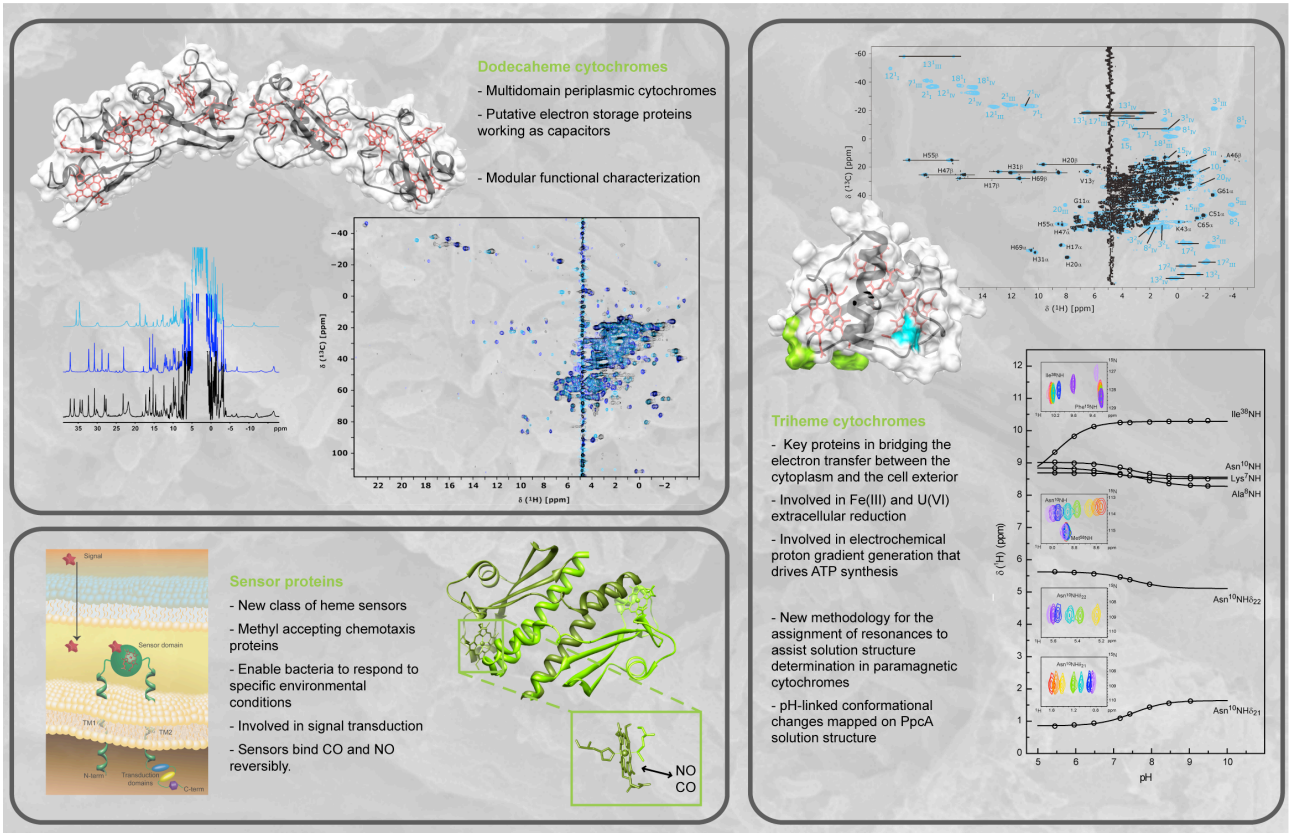


Figure 1 – Main NMR-based achievements on the targeted biological systems under study at Biochemistry and Bioenergetics of Heme Proteins group at Requimte-CQFB (FCT/UNL)

Structural information on these systems in solution is also crucial to understand their functional mechanisms. However, in the case of multiheme cytochromes, the traditional NMR based-protocols are extremely time-consuming, preventing a timely and successful characterization of heme proteins. The presence of numerous proton-containing groups in the heme cofactors and the magnetic properties of the heme iron, in particularly in the oxidized state, complicate signifi-

cantly the assignment of the NMR signals. As a consequence, the multiheme proteins super-family is extremely under-represented in structural databases, which constitutes a severe bottleneck in the elucidation of their structural-functional relationships. New NMR-based methodologies were developed by our group to study heme proteins, by combining a cost-effective isotopic labeling of the protein polypeptide chains and the comparative analysis of ^{1}H-^{13}C HSQC NMR spectra obtained for labeled and unlabeled samples.[5-6] These methodologies allow a straight discrimination between the heme cofactors and the polypeptide chain signals and their confident assignment.
The new NMR-based methodologies have been used to functional and structurally study several *Gs* heme proteins. [4-5, 7-12] The main results obtained are summarized in the figure. Overall, the methodologies are expected to constitute a promising strategy to guide the design of newly engineered *Gs* cytochromes for the improvement of the bioremediation and electricity harvesting skills of *Gs*.

Funding

This work is supported by grants PTDC/BIA-PRO/74498/2006, PTDC/QUI/70182/2006 and PEst-C/EQB/LA0006/2011 from Fundação para a Ciência e a Tecnologia (FCT, Portugal). LM and MAS are recipient of grants SFRH/BD/37415/2007 and SFRH/BD/61952/2009, respectively. The NMR spectrometers are part of the National NMR Network (RNRMN) and are funded by FCT.

References

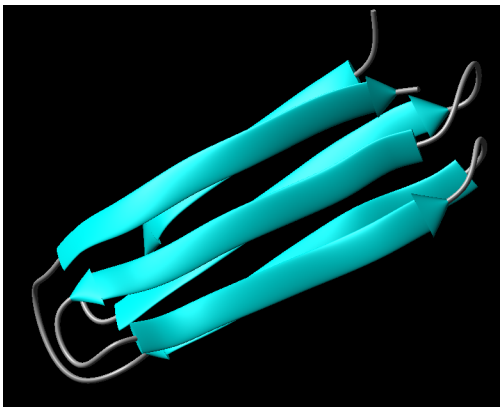
[1] Lovley DR, Ueki T, Zhang T, Malvankar NS, Shrestha PM, Flanagan KA, et al., "*Geobacter*: The Microbe Electric's Physiology, Ecology, and Practical Applications." *Adv Microb Physiol* **2011,** 59, 1-100.
[2] Shelobolina ES, Coppi MV, Korenevsky AA, Didonato LN, Sullivan SA, Konishi H, et al., "Importance of *c*-type cytochromes for U(VI) reduction by *Geobacter sulfurreducens*." *BMC Microbiol* **2007,** 7, 16.
[3] Methé BA, Nelson KE, Eisen JA, Paulsen IT, Nelson W, Heidelberg JF, et al., "Genome of *Geobacter sulfurreducens*: metal reduction in subsurface environments." *Science* **2003,** 302, 1967-9.
[4] Morgado L, Bruix M, Pessanha M, Londer YY, Salgueiro CA, "Thermodynamic characterization of a triheme cytochrome family from *Geobacter sulfurreducens* reveals mechanistic and functional diversity." *Biophys J* **2010,** 99, 293-301.
[5] Morgado L, Fernandes AP, Londer YY, Bruix M, Salgueiro CA, "One simple step in the identification of the cofactors signals, one giant leap for the solution structure determination of multiheme proteins." *Biochem Biophys Res Commun* **2010,** 393, 466-70.
[6] Fernandes AP, Couto I, Morgado L, Londer YY, Salgueiro CA, "Isotopic labeling of *c*-type multiheme cytochromes overexpressed in *E. coli*." *Prot Expr Purif* **2008,** 59, 182-188.
[7] Catarino T, Pessanha M, De Candia AG, Gouveia Z, Fernandes AP, Pokkuluri PR, et al., "Probing the chemotaxis periplasmic sensor domains from *Geobacter sulfurreducens* by combined resonance Raman and molecular dynamic approaches: NO and CO sensing." *J Phys Chem B* **2010,** 114, 11251-60.
[8] Dantas JM, Morgado L, Londer YY, Fernandes AP, Louro RO, Pokkuluri PR, et al., "Pivotal role of the strictly conserved aromatic residue F15 in the cytochrome c_7 family." *J Biol Inorg Chem* **2012,** 17, 11-24.
[9] Morgado L, Bruix M, Orshonsky V, Londer YY, Duke NE, Yang X, et al., "Structural insights into the modulation of the redox properties of two *Geobacter sulfurreducens* homologous triheme cytochromes." *Biochim Biophys Acta* **2008,** 1777, 1157-65.
[10] Morgado L, Fernandes AP, Londer YY, Pokkuluri PR, Schiffer M, Salgueiro CA, "Thermodynamic characterization of the redox centres in a representative domain of a novel *c*-type multihaem cytochrome." *Biochem J* **2009,** 420, 485-92.
[11] Morgado L, Paixão VB, Salgueiro CA, Bruix M, "Backbone, side chain and heme resonance assignments of the triheme cytochrome PpcA from *Geobacter sulfurreducens*." *Biomol NMR Assign* **2011,** 5, 113-16.
[12] Morgado L, Paixao VB, Schiffer M, Pokkuluri PR, Bruix M, Salgueiro CA, "Revealing the structural origin of the redox-Bohr effect: the first solution structure of a cytochrome from *Geobacter sulfurreducens*." *Biochem J* **2012,** 441, 179-87.

Solution structure of a metastable antibiotic

David L. Turner[1], Pedro Lamosa[1], and Beatriz Martinez[2]

[1]Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Av. da República – EAN, 2780-157 Oeiras, Portugal. [2]Instituto de Productos Lácteos de Asturias (IPLA-CSIC), Villaviciosa, Asturias, Spain.

Lactococcus lactis subsp. lactis IPLA972 is a wild lactococcal strain suitable for use in the manufacture of dairy products; it was characterised at the Instituto de Productos Lácteos de Asturias, Spain. This strain produces a unique bacteriocin, lactococcin 972 (Lcn972), comprising 66 aminoacids that blocks septum formation in dividing cells. Lcn972 also targets lipid II and competes with nisin, but it does not form pores in the membrane [1]. A detailed understanding of the interaction between Lcn972 and lipid II could suggest ways to improve antibiotics such as vancomycin and ramoplanin.
Attempts to crystallise Lcn972 for X-ray diffraction have been unsuccessful and so this work presents the structure determined in solution by NMR methods as a step towards finding its mode of action.
NMR also showed that Lcn972 is unusually rigid despite its small size and lack of cross links; some extreme proton chemical shifts indicate a lack of motional averaging in the vicinity of aromatic sidechains. The resulting structure is very well defined with an unusually compact sandwich of three-stranded beta sheets. The first layer comprises strands 1, 2 and 5, and the second layer comprises strands 4, 3 and 6. If the hydrogen bonds between strands 3 and 6 are broken, the sandwich can unfold.



Acknowledgments

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Reference

[1] Martínez B, Suárez JE & Rodríguez A (1996) Lactococcin 972, a homodimeric lactococcal bacteriocin whose primary target is not the plasma membrane. *Microbiology* 142, 2393-2398.

Material Sciences and SSNMR

Quantifying weak packing interactions in the antibiotic ciprofloxacin: a combined solid-state NMR, X-ray diffraction and computational study

Mafra L,[a, b] Santos SM,[a] Siegel R,[a] Alves I,[a] Paz FAA,[a] Dudenko D,[b] Spiess HW[b]

[a]*Department of Chemistry, University of Aveiro, CICECO, Campus de Santiago, 3810-193 Aveiro, Portugal.*
[b]*Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany*

In pharmaceuticals crystallization and formulation processes both, understanding the effect of water on the transformation of drug hydrates to anhydrates, and exploring the correlations between the water environment in the crystal lattice and the hydration and dehydration behavior, are non-trivial matters of particular concern. In this regard, hydrogen bonding and van der Waals interactions are considered to play major roles as structure-driving entities in the construction of supramolecular arrangements. This is of particular relevance in pharmaceutical sciences, as multiple crystal forms of the same active pharmaceutical ingredient (API) occur frequently, posing diverse problems in the pharmacokinetics, stability, and formulation of drugs. In particular, pharmaceutical hydrates represent a class of multiple-component crystals of great relevance, often exhibiting a well-defined stoichiometric relation between the water and the parent molecule. In other cases water may be removed non-stoichiometrically, yielding multiple hydrate forms until the anhydrate forms. At present, we are far from fully understanding the drug hydration-dehydration processes. The use of reliable methodology for the identification and characterization of polymorphs and hydrates is therefore a field of great importance and much research efforts. In recent years, the use of solid-state NMR spectroscopy in tandem with computational approaches based on periodic boundary conditions to calculate NMR parameters, has come to the fore, showing much potential in various applications involving the study of small molecules. NMR chemical shifts depend on the electronic environment of the nucleus studied. This gives us the unique opportunity to quantify the effect of the molecular packing on the chemical shifts in drug hydrate systems. Our contribution reports a first step in quantifying the energetics of the different contributions to the crystal packing by in silico computer simulation.[1]

In an attempt to better understand how drug hydrates self-assemble in the solid-state and reorganizes to produce its anhydrous form, we present an experimental NMR, X-ray diffraction (XRD), and computational study of the supramolecular assemblies of two crystalline forms of the antibiotic ciprofloxacin (CIP): one anhydrate (form I) and one hydrate (form II) forming water wormholes (Figure 1), emphasizing the effect of nonconventional hydrogen bonds and water on NMR chemical shifts. The complete resonance assignment of up to 51 and 54 distinct 13C and 1H resonances for the hydrate is reported, using a toolbox of advanced high-resolution 2D 1H CRAMPS-based NMR experiments and high magnetic fields (Figure 2) combined with GIPAW calculations of 1H/13C chemical shifts (Figure 3). The effect of crystal packing on the 1H and 13C NMR chemical shifts including weak interionic hydrogen bonds and π···π interactions, is quantified through in silico structure dismantlement of I and II (Figure 3). For example, 1H chemical shift changes up to ~–3.5 ppm for CH···π contacts and ~ +2 ppm (CH···O(–)); ~+4.7 ppm ((+)NH···O(–)) were estimated for hydrogen bonds.[1] Water intake induces chemical shift changes up to 2 and 5 ppm for 1H and 13C nuclei, respectively. We show that such chemical shifts are found to be sensitive detectors of hydration/dehydration in the highly insoluble CIP hydrates.[1]

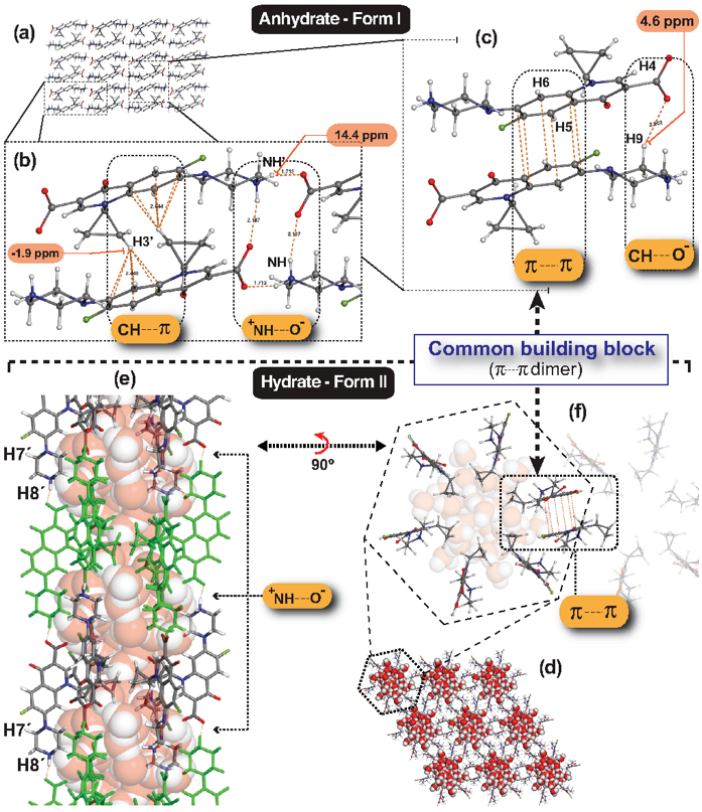

Figure 1 – Crystal packing overview of **I** (top) and **II** (bottom) CIP forms showing (a, d) the full crystallographic arrangement along one of its axes directions and (c–f) the detailed views outlining specific packing interactions. (b) CIP tetramer involving two CH···π dimers; (c, f) a CIP π···π dimer; (e) water channel surrounded by six 1D CIP molecular chains connected through $^{(+)}$N···H$^{(-)}$ H-bonds. For the sake of clarity CIP residues are shown in alternated colors in (e).

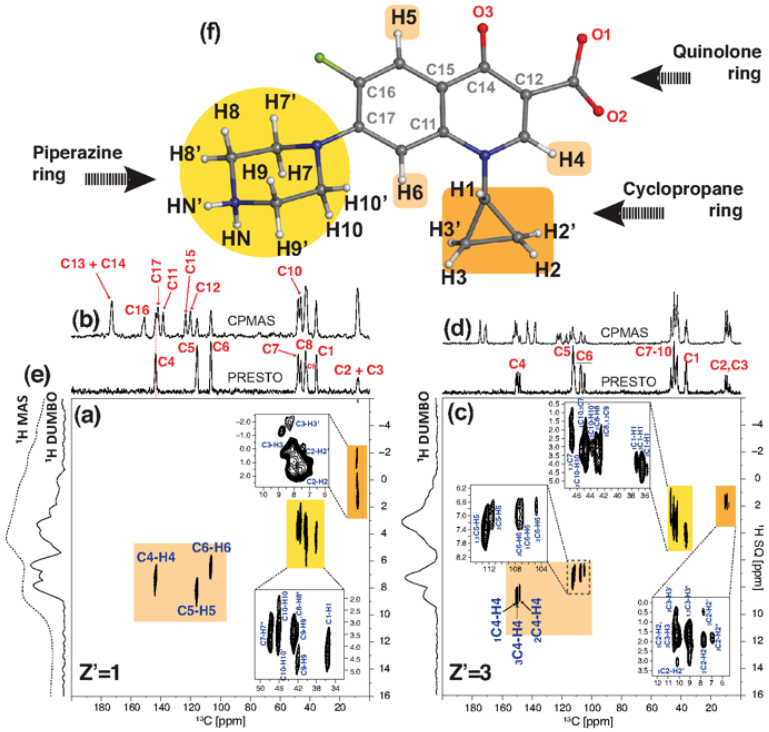

Figure 2 – 2D ^{1}H–^{13}C PRESTO-HETCOR of CIP forms (a) I and (c) II recorded at 800 MHz. (b, d) ^{13}C CPMAS spectra recorded at 400 MHz. (e) ^{1}H MAS and wDUMBO spectra of I are shown for comparison with the F1 projection of (a). (f) Labeling scheme adopted for CIP. The capability of PRESTO transfer to select only the directly bonded C– H is manifested by comparison with the ^{13}C CPMAS spectra [i.e., (a, c) vs (b, d)].

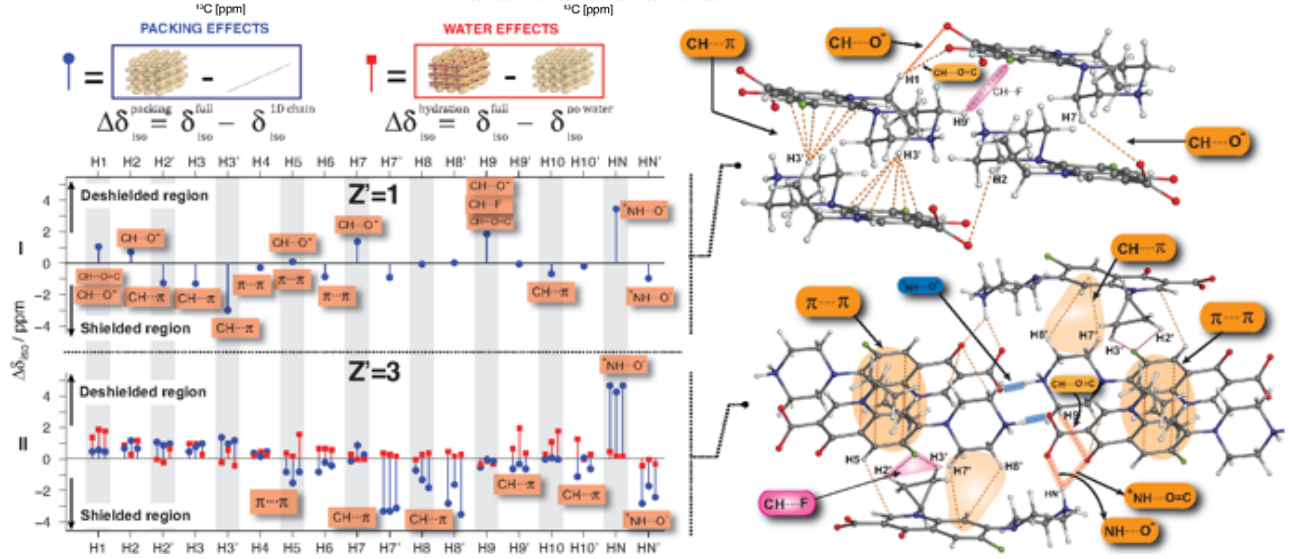

Figure 3 – (Left) Stem plots showing the contribution of the crystal packing (blue stems) and water molecules (red stems) to the calculated ^{1}H chemical shifts (positive Δδ values indicate low-field shifts) of the ciprofloxacin forms **I** and **II**. In **II**, each of the three stems per nuclei corresponds to the crystallographically distinct CIP molecules 1, 2, and 3 (from left to right); (right) detailed view of intermolecular interactions in packings of **I** and **II**.

Funding

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References

[1] Mafra L, Santos SM, Siegel R, Alves I, Paz FAA, Dudenko D, Spiess HW, "Packing interactions in hydrated and anhydrous forms of the antibiotic ciprofloxacin: a solid-state NMR, X-ray diffraction, and computer simulation study", *Journal of the American Chemical Society* **2012**, in press, DOI: 10.1021/ja208647n945-954.

Solid-state NMR studies on the molecular dynamics of amorphous Simvastatin

Teresa G. Nunes[a], M. Teresa Viciosa[b], Hermínio P. Diogo[a]

[a]Centro de Química Estrutural; [b]Centro de Química-Física Molecular
Instituto Superior Técnico/Univ. Técnica Lisboa, Av. Rovisco Pais 1049-001 Lisboa, Portugal

The growing number of active pharmaceutical ingredients (APIs) with poor aqueous solubility has led to converting crystalline drug compounds to their amorphous forms as one of the most promising tools. API has higher efficiency when has good bioavailability and ultimately good dissolution, solubility in human fluids and good permeability in gastrointestinal tract. Thus, methods for stabilization of amorphous forms of drugs are emerging.[1]
Simvastatin (Fig.1a) is a cholesterol-lowering agent commonly used to treat hypercholesterolemia; it has three crystalline polymorphs with well-defined temperature regions (enantiotropic system).[2] The Form I is used in pharmacology and it is characterized by very low solubility and therefore low oral bioavailability. The use of amorphous simvastatin requires controlling devitrification but the evaluation of molecular dynamics is also important because rigid glassy APIs are mostly required. Solid-state NMR spectroscopy was the technique chosen for both purposes because is particularly valuable to probe short-range order and to study molecular dynamics under different frequency ranges.
Amorphous simvastatin sample was produced by the quenched cooled method: heated at 10 K/min up to 423 K and immediately cooled down below the glass transition temperature. No cold crystallization signals were detected up to 350 K by DSC. Conventional MAS ^{1}H and ^{13}C CP techniques were used over 293 K and 333 K, and line shape simulations were performed as previously described.[3] The spin-lattice in the rotating frame of carbon nuclei ($^{C}T_{1\rho}$) was measured to evaluate dynamics in the 10-100 kHz frequency range.

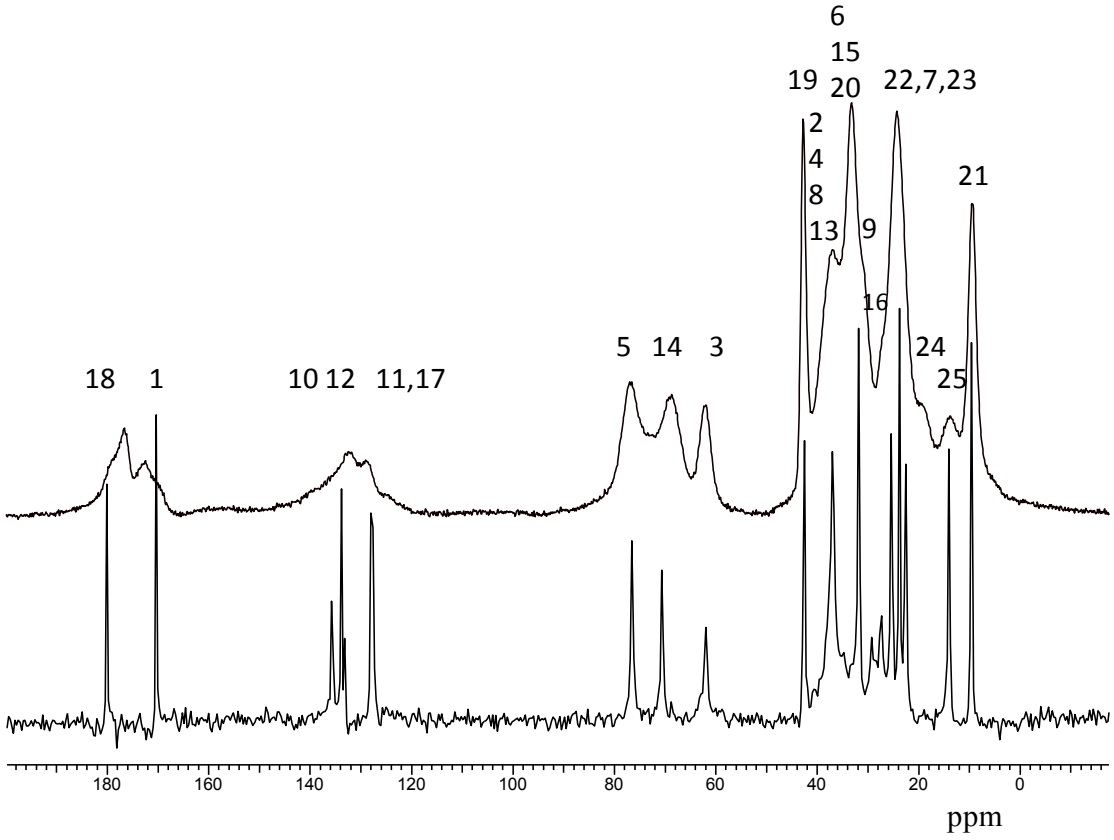

Figure 1. a) Structural formula of simvastatin. b) ^{13}C CP/MAS spectra obtained from different simvastatin samples using the SELTICS sequence: crystalline (bottom) and amorphous (top).

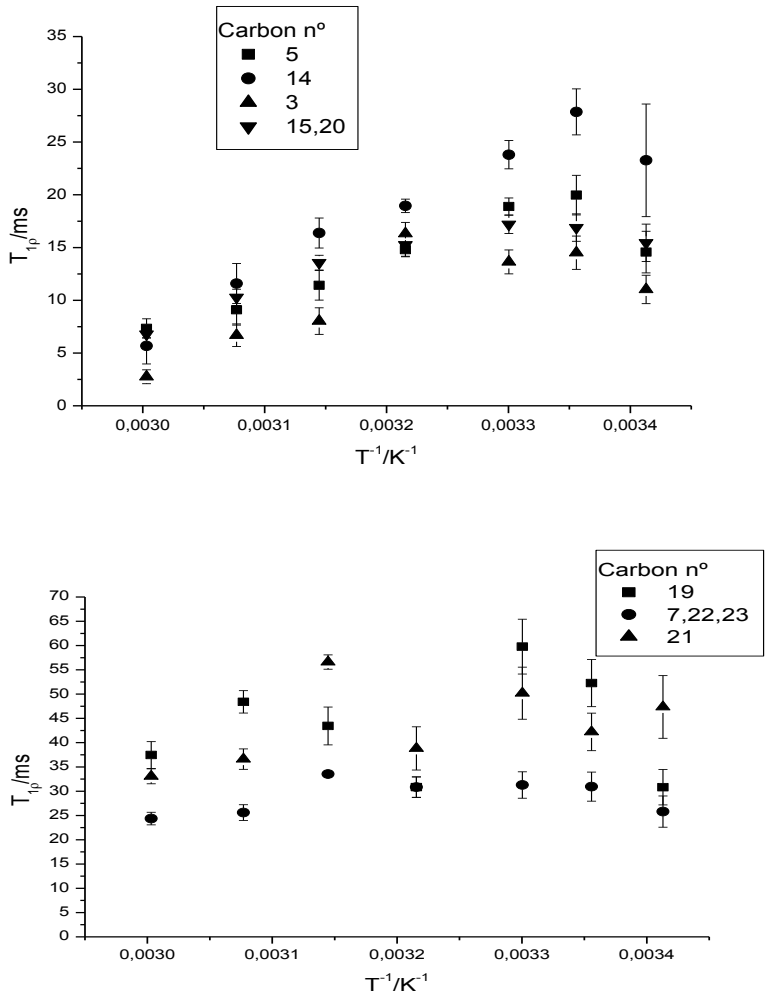

Figure 2. Spin-lattice relaxation time in the rotating frame of the indicated carbon atoms measured from 293 till 333 K.

The results show that dipole-dipole interaction is the driven mechanism for spin-lattice relaxation in the rotating frame; quaternary and methyl carbons present higher $^{C}T_{1\rho}$. Cooperative torsional oscillations of the rings explain the observed $^{C}T_{1\rho}$ decrease at $T > T_g$.

^{1}H data are consistent with motion of hydroxyl groups being observed. The strong line narrowing of the resonance at higher frequency is in agreement with a decrease of the correlation time when the sample is heated up most probably due to reorientation between sites C3(O-H...OC18) and C18(O-H…OC3).

The present study demonstrated that crystalline simvastatin could be physically transformed to its amorphous form using the quenched cooled method without any chemical degradation thus revealing important potential application of the glassy API from the formulation point of view.

Funding

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References

1. R. Laitinen, K. Löbmann, CJ. Strachan, H. Grohganz, and T. Rades, *Int. J. Pharm.* (in press)
2. M. Hušák, B. Kratochvíl, A. Jegorov, J. Brus, J. Maixner, and J. Rohlíček, *Struct. Chem.,* **2010**, 21, 511-18.
3. TG. Nunes, HP. Diogo, S. Pinto, and JJ. Moura Ramos. *J. Phys. Chem.B,* **2010**, 114, 15976-84.

Small molecules

(structure, dynamics and interaction)

Structure elucidation of synthetic antioxidant agents by NMR: Polyhydroxyxanthones

Silva A.[1], Santos C.[2]

[1]*Department of Chemistry &QOPNA, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal*

[2]*Polytechnic Institute of Bragança, School of Agriculture, Department of Vegetal Production and Technology, 5301-855 Bragança, Portugal*

Xanthones are a class of oxygen-containing heterocyclic compounds widely distributed in nature. Over the last decades these compounds have been extensively studied not only because they participate in several biological functions but also due to their remarkable biological activities, namely as promising antioxidant agents. Structure–activity studies of phenolic compounds have revealed that features conducive to high antioxidant activity are the presence of hydroxyl groups at certain positions on the skeleton, a catechol group being the most prominent moiety. In view of these considerations, we have reported two main routes for the synthesis of polyhydroxylated 2,3-diaryl-9*H*-xanthen-9-ones.[1] The ROS and RNS scavenging activity evaluation of these new 2,3-diarylxanthones revealed that they possess outstanding scavenging properties, considering the nanomolar to micromolar range of the IC50 values found. The xanthone with two catechol rings was the most potent scavengers of all tested ROS and RNS.[2]

NMR spectroscopy is an extremely powerful tool in the structural elucidation of small organic molecules, namely by establishing their carbon skeleton and also to establish their stereochemistry. In the synthesis of the referred polyhydroxylated 2,3-diaryl-9*H*-xanthen-9-ones the 1D (^{1}H, ^{13}C) and 2D (HSQC, HMBC, NOESY) NMR techniques were extremely useful in the structure determination of all intermediates and final products (Figure 1 and 2). Specifically NOESY spectra allowed us to unequivocally prove the stereochemistry of some intermediates, namely those having several double bonds (Figure 2).[2]

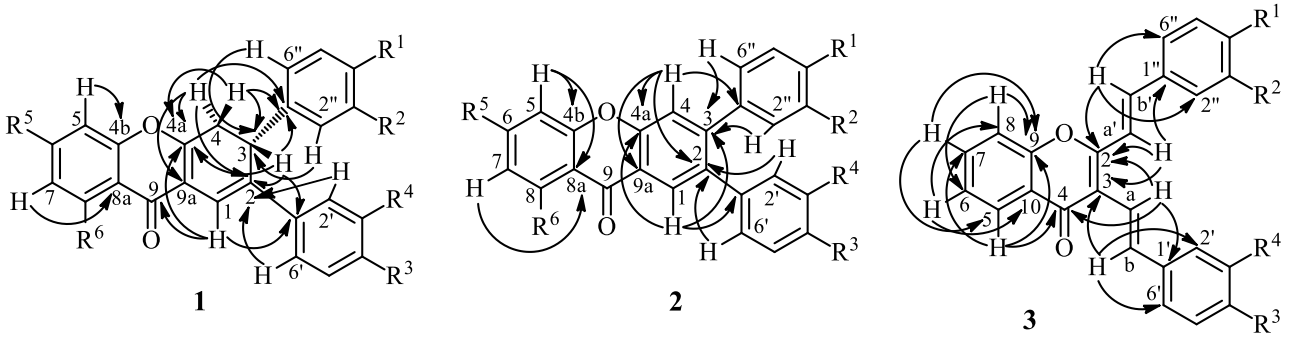

Figure 1. Important connectivities found in the HMBC spectra of 2,3-diaryl-3,4-dihydro-9*H*-xanthen-9-ones **1**, 2,3-diaryl-9*H*-xanthen-9-ones **2** and (*E*,*E*)-2,3-distyryl-4*H*-chromen-4-ones **3**.

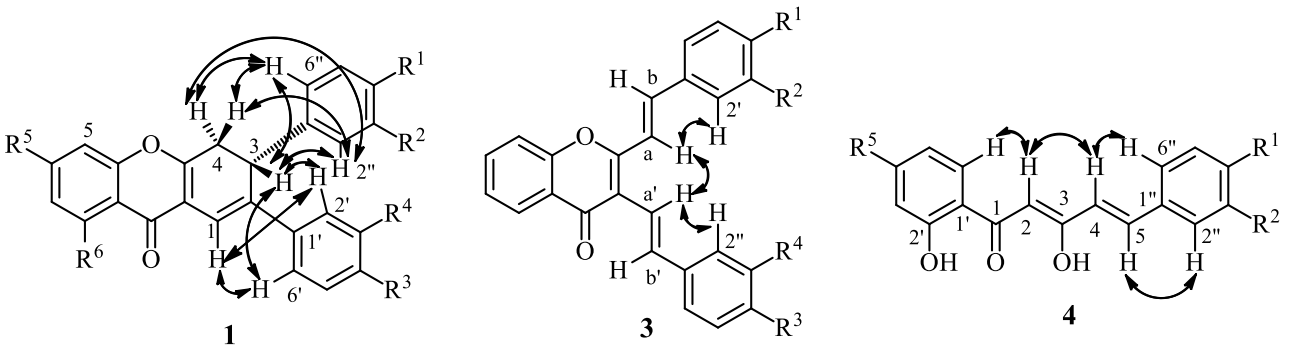

Figure 2. Main NOE cross peaks found in the NOESY spectra of 2,3-diaryl-3,4-dihydro-9*H*-xanthen-9-ones **1**, (*E*,*E*)-2,3-distyryl-4*H*-chromen-4-ones **2** and 5-aryl-3-hydroxy-1-(2-hydroxyphenyl)penta-2,4-dien-1-ones **4**.

Funding

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References

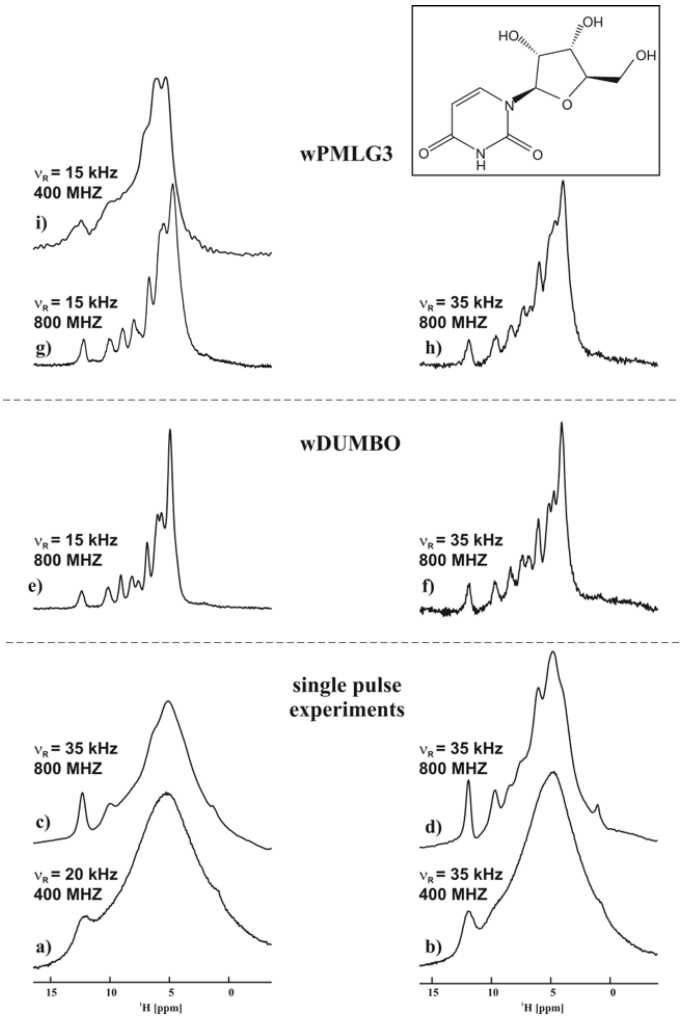
1. Santos CMM, Silva AMS, Cavaleiro JAS, "Efficient Syntheses of New Polyhydroxylated 2,3-Diaryl-9H-xanthen-9-ones", *European Journal of Organic Chemistry* **2009**, 2642-2660.
2. Santos CMM, Freitas M, Ribeiro D, Gomes A, Silva AMS, Cavaleiro JAS, Fernandes E, "2,3-Diarylxanthones as strong scavengers of reactive oxygen and nitrogen species: A structure–activity relationship study", ***Bioorganic & Medicinal Chemistry*** **2010**, 18, 6776–6784.

High-resolution ^{1}H NMR techniques for the study of solids

Mafra L, Siegel R, Rocha J.

Department of Chemistry, University of Aveiro, CICECO, Campus de Santiago, 3810-193 Aveiro, Portugal

^{1}H NMR spectroscopy is an extremely powerful and now routine tool for studying molecular structure and dynamics in liquids. In contrast, investigating solids by ^{1}H NMR still presents considerable challenges because the strong ^{1}H–^{1}H dipolar coupling (dominant interaction in rigid solids) homogeneously broadens the proton resonances up to a few tens of kHz. The ^{1}H homonuclear dipolar interaction may be partially averaged out using NMR techniques developed since the sixties, which rely on two strategies: (i) periodic radio-frequency (rf) multiple-pulse sequences, acting on the spin part; (ii) magic-angle spinning (MAS) to average the spatial part. Both come together in the so-called Combined Rotation and Multiple-Pulse Spectroscopy (CRAMPS). Recent technological developments in NMR probes (MAS up to 70 kHz) and spectrometer consoles (fast electronics) contributed to a considerable improvement in the quality and resolution of ^{1}H NMR spectra. Although much of the NMR community considered that 1H decoupling would not work at very fast MAS rates, we have shown recently that DUMBO and PMLG 1H homonuclear decoupling techniques perform well at MAS rates up to 35 kHz and magnetic fields of 9.4 and 18.8 T.1 As an example, Figure 1 shows the ^{1}H spectra of uridine, a biological solid.[1]



Double-quantum (DQ) homonuclear recoupling MAS NMR methods are among the most useful techniques available to chemists. Such techniques encode important structural information by restoring the through-space dipole–dipole couplings, such as distance information between interacting nuclei. They also allow estimating torsional angles, filtering signals of mobile or isolated spin species and provide a route to the excitation of higher coherence orders. In addition, the availability of CRAMPS decoupling techniques capable of performing well at very fast MAS, opens up new perspectives in ^{1}H NMR spectroscopy, providing improved resolution in 2D ^{1}H-^{1}H DQ–SQ correlation experiments. Most DQ ^{1}H recoupling techniques are mainly confined to moderate MAS rates (10–15 kHz) because the recoupling part of the sequence requires very large rf field strengths. We have recently shown that R rotor-synchronised sequences allow efficient ^{1}H–^{1}H DQ recoupling at MAS rates up to 67 kHz, thus overcoming the difficulties of obtaining high-quality ^{1}H spectra at fast MAS rates. Although R sequences have already been used to recouple ^{13}C–^{13}C dipolar interactions at MAS rates below 22 kHz, our contribution is the first work showing the capability to reintroduce ^{1}H–^{1}H dipolar couplings at ultrafast spinning rates (67 kHz).[2] The method was illustrated on two solids of biological interest, amino-acid tyrosine hydrochloride (Tyr·HCl) and tri-peptide glutathione in its reduced form (GSH), at magnetic fields of 14.1 and 18.8 T. ^{1}H homonuclear decoupling (DUMBO) is employed in the DQ (t1) and SQ (t2) dimensions using the pulse sequence depicted in Figure 2.

Figure 1 – ^{1}H NMR spectra of uridine recorded employing (a–d) ^{1}H single-pulse excitation (SPE); wDUMBO decoupling using (e) ν_1 = 112 kHz, (f) ν_1 = 146 kHz; wPMLG3 decoupling using (g) ν_1 = 112 kHz, (h) ν_1 = 146 kHz and (i) ν_1 = 70 kHz. Recycle delay: 25 s. The experimental scaling factors were (e) λ_{exp} = 0.61; (f) λ_{exp} = 0.61; (g) λ_{exp} = 0.65; (h) λ_{exp} = 0.73 and (i) λ_{exp} = 0.69.

The achieved 2D high-resolution ^{1}H DQ-SQ homonuclear correlation spectrum of Tyr·HCl combining such ^{1}H decoupling and ultra-fast MAS shows an outstanding resolution enhancement, allowing its full assignment and the distinction between intra- and inter-molecular ^{1}H proximities (Figure 3).[2]

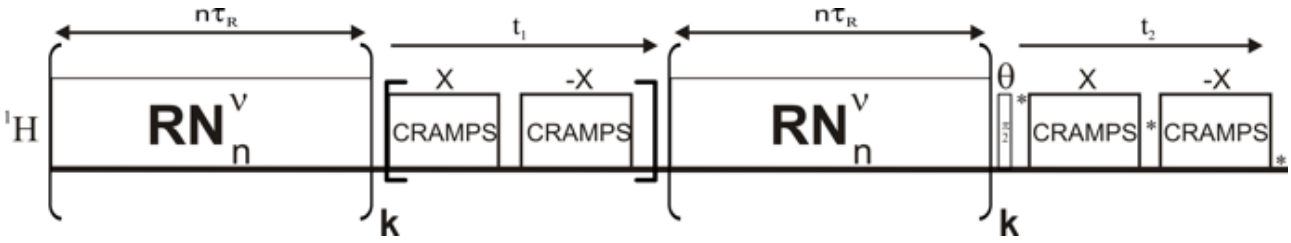


Figure 2 – Pulse sequence for 2D ^{1}H-^{1}H DQ homonuclear recoupling experiments. and symmetries are used for DQ excitation/reconversion (k=1). Here, we use the CRAMPS decoupling scheme DUMBO during the t_1 and t_2 evolutions. The flip angle of the read pulse is θ=90°. ??? recoupling blocks are of the form ???? where ???? (the rf phase in degrees) and the basic element R is a 180° flip angle. Therefore, for sequences employing a complete ??? recoupling six pairs of building blocks of the type ???? were employed, which gives a total of 12 R pulses spanning over two rotor periods during the excitation and reconversion blocks because n=2. In the same way, ??? recoupling employs a ???? building block spanning over four rotor periods (n=4). The nutation frequency (ν_1) for any of the RN sequences is detailed in Table 1 and may be calculated using the expression $\nu_1=(N/2n)*\nu_R$

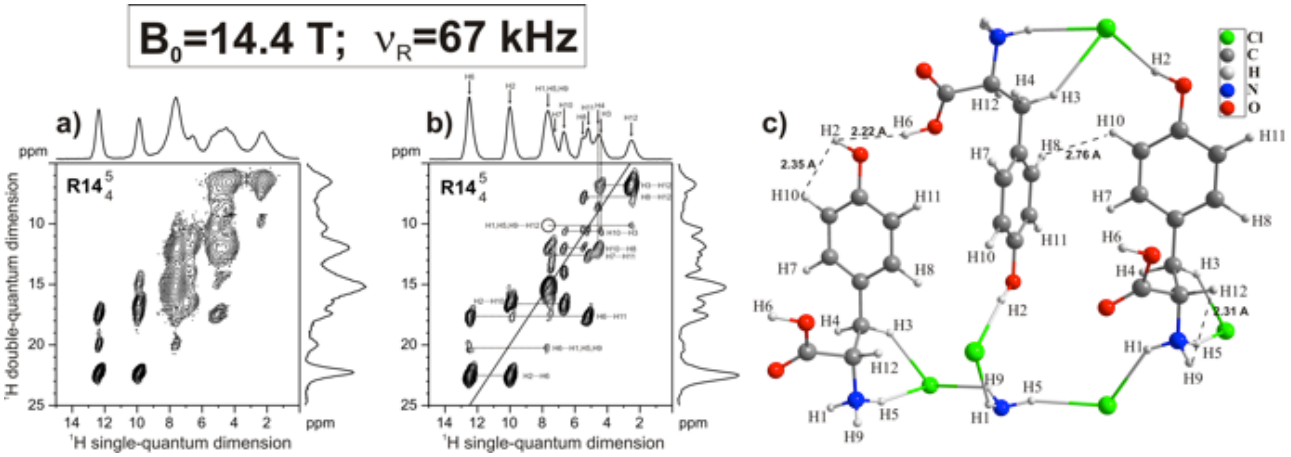


Figure 3 – 2D ^{1}H-^{1}H DQ-SQ spectra of Tyr.HCl, recorded at MAS 67 kHz using ν_1=117 kHz and Larmor frequency of 600 MHz (B_0=14.1 T, Bruker wide-bore NMR spectrometer), using the symmetry ??? for ^{1}H-^{1}H recoupling. a) No CRAMPS used, b) DUMBO decoupling in both dimensions (DUMBO shape pulse length = 15 μs; Decoupling power=198 kHz), c) Schematic representation of the solid-state structure of Tyr.HCl.

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References

[1] Mafra L, Coelho C, Siegel R, Rocha J, "Assessing the performance of windowed H-1 CRAMPS methods, on biological solids, at high-field and MAS up to 35 kHz", *Journal of Magnetic Resonance* **2009**, 197, 20-27
[2] Mafra L, Siegel R, Fernandez C, Schneider D, Aussenac F, Rocha J, High-resolution H-1 homonuclear dipolar recoupling NMR spectra of biological solids at MAS rates up to 67 kHz, *Journal of Magnetic Resonance* **2009**, 199, 111-114

Structural elucidation of drug metabolites and covalent drug-protein adducts by NMR

Marques MM, Antunes AMM

Centro de Química Estrutural, Instituto Superior Técnico, Universidade Técnica de Lisboa, 1049-001 Lisboa, Portugal

Drugs, as any other xenobiotics, undergo biotransformation to more hydrophilic derivatives, so that excretion can occur. However, metabolic pathways can also be responsible for the formation of reactive (primarily electrophilic) species capable of reacting with biomacromolecules to afford covalent protein and DNA adducts that may elicit direct cell toxicity, trigger an immune response and/or initiate mutagenicity/carcinogenicity. Drug bioactivation is, therefore, a frequent event at the onset of drug-induced toxicity.

As part of our program aimed at studying the long-term toxic effects induced by anti-HIV drugs we have explored several NMR experimental approaches. Much of our work relies on the synthesis and structural characterization of drug metabolites, protein and DNA adducts (biomarkers of toxicity) to be used as standards to test their formation *in vivo*, in animal models and in humans. Hence, reliable standards are only possible upon full structural elucidation and NMR is a major tool in this context, with ample use of classical gradient fields, homo- and heteronuclear 2D experiments, and selective pulse-based experiments.[1-4] Indeed, these techniques were extremely useful for the structural elucidation of both metabolites (*eg.,* **1** and **2**, **Figure 1**) and covalent amino acid adduct standards (*eg.,* **3** and **4**) of the anti-HIV drugs nevirapine and abacavir.

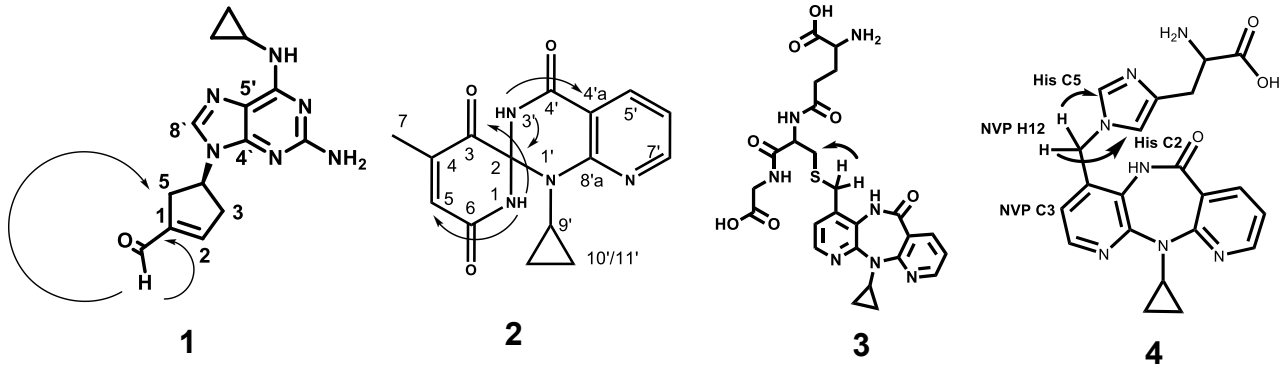

Figure 1. Important connectivities observed in the HMBC spectra of the abacavir metabolite, conjugated aldehyde (**1**), the spiro product (**2**), obtained upon hydrolysis of a quinone-imine derivative of nevirapine, and the nevirapine adducts 12-(glutathion-*S*-yl)-nevirapine (**3**) and 12-(histidin-*N*1'-yl)-nevirapine (**4**). Of note is the fact that for adduct **4** these connectivies were only observed upon use of a semi-selective HMBC pulse program, while for the assignment of all resonances of adduct **3** the HSQC-TOCSY experiment was essential.

In addition, taking advantage of the presence of a fluoro substituent in the anti-HIV drug Efavirenz, we are currently exploring ^{19}F NMR to study the interaction of efavirenz with the transport protein Human Serum albumin.[5] These studies are of great interest to evaluate drug-drug interactions at HSA levels, which is particularly important for efavirenz which is a drug with a narrow therapeutic window.

Funding

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References

1. Antunes AMM, Novais D, Ferreira da Silva JL, Santos PP, Oliveira MC, Beland FA, Marques MM, Synthesis and oxidation of 2-hydroxynevirapine, a metabolite of the HIV reverse transcriptase inhibitor nevirapine, *Org. Biomol. Chem.* **2011**, 9, 7822-7835.
2. Charneira C, Godinho ALA, Oliveira MC, Pereira SA, Monteiro EC, Marques MM, Antunes AMM, Reactive Aldehyde Metabolites from the Anti-HIV Drug Abacavir: Amino Acid Adducts as Possible Factors in Abacavir Toxicity, *Chem. Res. Toxicol.* **2011**, 24, 2129-2141.
3. Antunes AMM, Godinho ALA, Martins IL, Justino GC, Beland FA, Marques MM, Amino acid adduct formation by the nevirapine metabolite, 12-hydroxynevirapine – a possible factor in nevirapine toxicity, *Chem Res Toxicol.* 2010, 23, 888–899.
4. Antunes AMM, Duarte MP, Santos, PP, Gamboa da Costa G, Heinze TM, Beland FA, Marques MM, Synthesis and Characterization of DNA Adducts from the HIV Reverse Transcriptase Inhibitor Nevirapine, *Chem Res Toxicol*, **2008**, 21, 1443–1456.
5. Wanke R, Harjivan SG, Marques MM, Antunes AMM, Binding of the anti-HIV drug efavirenz to human serum albumin: a ^{19}F-NMR study, 244th ACS National Meeting & Exposition, Philadelphia, Pennsylvania, USA, **2012**. *Abstracts of Papers of the American Chemical Society* (in press).

NMR as a tool for the discovery of new anti-inflammatory drugs

Viegas A,[a] Estevão MS,[a] Carvalho LC,[a] Freitas M,[b] Gomes A,[b] Manso J,[a] Erhardt S,[a] Fernandes E,[b] Marques MMB,[a] Cabrita EJ[a]

[a]*REQUIMTE-CQFB, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal.*
[b]*REQUIMTE, Departamento de Química-Física, Faculdade de Farmácia, Universidade do Porto, Rua Aníbal Cunha, 164, 4099-030 Porto, Portugal.*

The anti-inflammatory and analgesic properties of non-steroidal anti-inflammatory drugs (NSAIDs) such as aspirin, ibuprofen or flurbiprofen are due to cyclooxigenase-2 (COX-2) inhibition, whereas side effects are associated with inhibition of COX-1. To overcome the side effects associated with COX-1 inhibition selective COX-2 inhibitors (coxibs) have been developed. However, the long-term use of both traditional NSAIDs and coxibs causes significant side effects and the development of selective inhibitors without side effects continues to stimulate the development of novel approaches towards selective anti-inflammatory drugs. In this context, in the past 3 years, we have successfully developed a NMR based approach, based on Saturation Transfer Difference (STD) NMR, to study the binding of small ligands to COX enzymes. Our work represents the first report of the use of NMR to investigate inhibition of COX enzymes.[1] STD-NMR is one of the most popular ligand-based NMR techniques for the study of protein-ligand interactions. This is a consequence of its robustness and the fact that it is focused on the signals of the ligand, using only small quantities of the nonlabeled receptor. STD-NMR can be used as a screening technique, for identification of lead structures, or for identifying ligand moieties important for binding.[2] To develop our methodology we applied STD-NMR to study the binding of ibuprofen to COX-1/COX-2 and ketorolac and diclofenac to COX-2. The study of the binding epitopes of ibuprofen and diclofenac with COX-2 together with STD competition experiments and comparison with the crystallographic structures allowed us to propose a binding mode for ketorolac similar to that of diclofenac with COX-2 (figure 1).

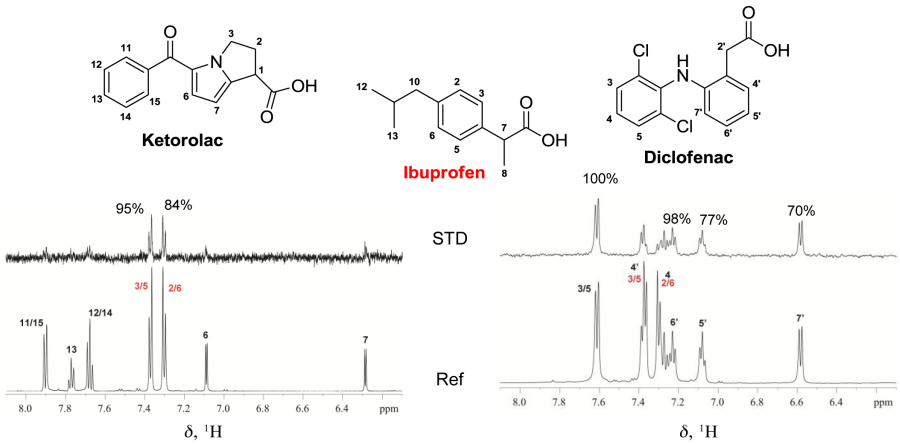

Figure 1. ^{1}H STD-NMR spectra of ibuprofen/ketorolac (left) and ibuprofen/diclofenac (right) in the presence of COX-2, at 600 MHz and 37 ºC.

The NMR methodology was then applied to a small library of new indolic compounds, involving two different substitutions patterns at the indole scaffold (figure 2), in order to establish a relation between the spatial distribution of known functional groups related with inhibitory activity. Inhibitory studies were performed and the activity results obtained against both COXs isoforms were rationalized based on docking and NMR studies. Docking studies showed that dialkyation at C-2 and C-3 favors a binding with an orientation similar to that of the known selective inhibitor SC-558. This substitution pattern is correlated with the highest inhibitory activity and selectivity: 70% COX-2 inhibition at 50 mM, and low COX-1 inhibition (18 ± 9%).

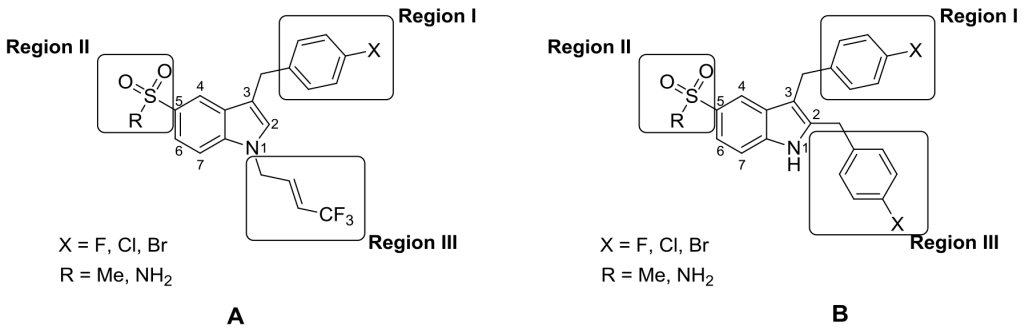

Figure 2 – Library approaches

The STD NMR experiments revealed different interaction patterns with both COXs isoforms that may be related with different orientations of the sulfonamide group in the binding pocket (figure 3).

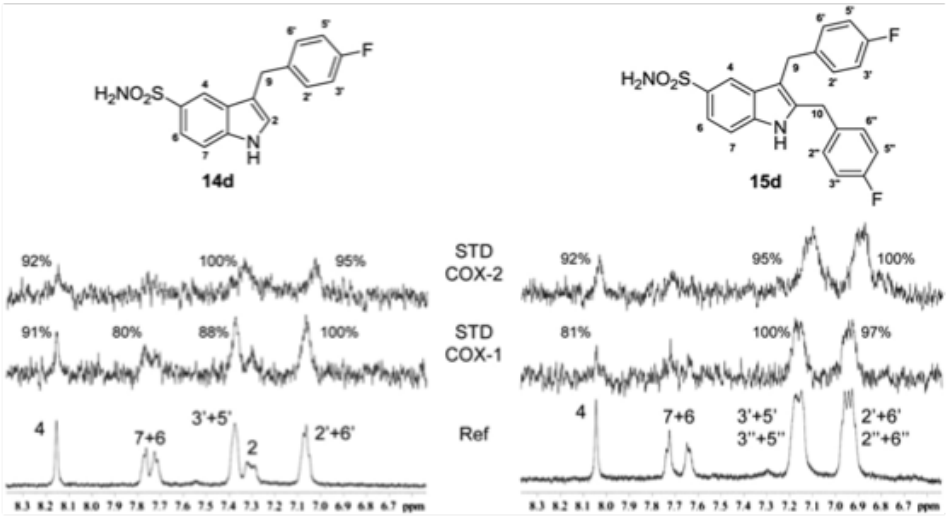

Figure 3 – STD NMR resuts

Despite the moderated inhibitory activities found, our study represents an innovative approach towards COXs inhibitory activity rationalization and to the design of anti-inflammatory drugs. The NMR methodology opened a new window of research to study the relation between multiple COX-2 binding sites, not only concerning inhibitors, but also other non-substrate molecules, like fatty acids.

Funding

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References

1. Viegas A, Manso J, Corvo MC, Marques MMB, Cabrita EJ "Binding of ibuprofen, ketorolac and diclofenac to COX-1 and COX-2 studied by saturation transfer difference NMR", *J. Med. Chem.* **2011**, 54, 8555-8562.

2. Viegas A, Manso J, Nobrega F, Cabrita EJ, "Saturation-Transfer Difference (STD) NMR – A simple and fast method for ligand screening and characterization of protein binding" *J. Chem. Ed*. **2011**, 88, 990-994.

3. Estevão MS, Carvalho LCR, Freitas M, Gomes M, Viegas A, Manso J, Erhadrt S, Cabrita EJ, Marques MMB "Indole based cyclooxygenase inhibitors: synthesis, biological evaluation, docking and NMR screening" *Eur. J. Med. Chem.* **2012**, 54, 823-833.

Poly(alkylidenamines) dendrimers as scaffolds for the preparation of low-generation ruthenium based metallodendrimers

Rodrigues J.[1], Jardim M. G.[1], Figueira J.[1], Gouveia M.[1], Tomás H.[1], Rissanen K.[2]
[1]CQM - Centro de Química da Madeira, MMRG, Universidade da Madeira, Campus Universitário da Penteada, 9000-390 Funchal, Portugal.
[2]NanoScience Center, Department of Chemistry, University of Jyväskylä, P. O. Box 35, 40014 JYU, Finland.

The aim of this research is to highlight the use of nitrile-functionalized poly(alkylidenamines) dendrimers as building blocks for the preparation of low-generation ruthenium based cationic metallodendrimers having in view potential biomedical applications. Air-stable poly(alkylidenamines) nitrile dendrimers, peripherally functionalized with the ruthenium moieties $[Ru(\eta^5\text{-}C_5H_5)(PPh_3)_2]^+$ or $[RuCl(dppe)_2]^+$, have been prepared, characterized and are being studied for their anticancer activity. The followed strategy is based on the biological advantages associated with low-generation dendrimers, the known activity of ruthenium compounds as anticancer drugs and the stability of these dendrimers at the physiological temperature.
One of the important aspects of drugs that are to be considered for biological tests and clinical applications is the knowledge of their degradation/stability in solution along the time, as well as of the type of species resulting from the degradation process. Time degradation studies of the prepared metallodendrimers were made using NMR spectroscopy (^{31}P NMR) by dissolving the prepared compounds in $[D_6]$ DMSO. The metallodendrimers were at the concentration of 0.019 mg μL^{-1} and, after a starting experiment at 25 °C, the NMR tube was incubated in a water bath at 37 °C at different time periods. ^{31}P NMR was performed to evaluate the degradation of the metallodendrimers/release of metallofragments.[1]

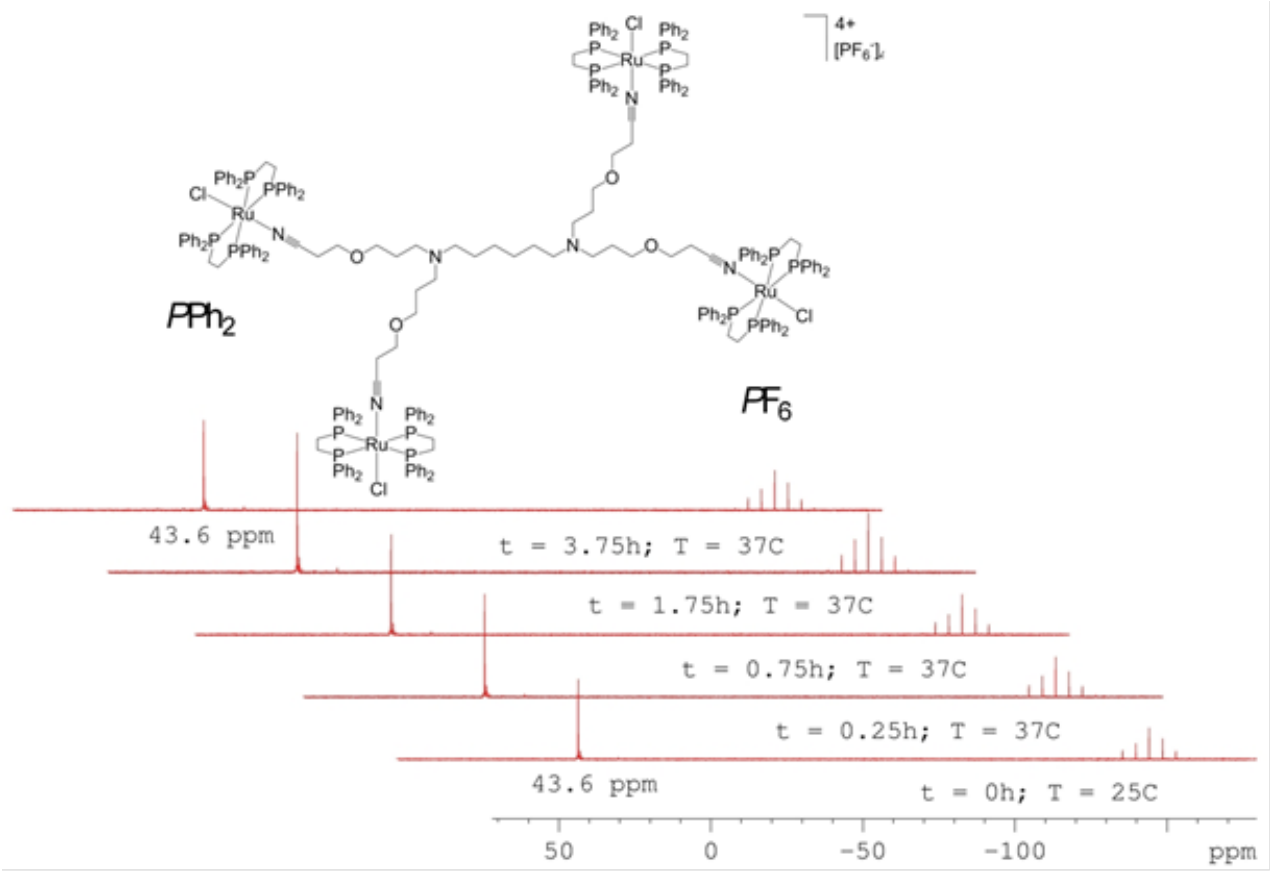

Figure 1. ^{31}P NMR spectrum of metallodendrimer in $[D_6]$ DMSO at 37°C at different time periods of incubation.

As far as we are aware, this series of five air-stable cationic zero generation ruthenium-based metallodendrimers was the first to be prepared and characterized using nitrile-functionalized poly(alkylidenamine) dendrimers. The degradation behavior of the metallodendrimers was studied by ^{31}P NMR in [D_6] DMSO, along the time, at physiological temperature, revealing the potential of the compounds to be studied for biomedical applications. Currently, the cytotoxic properties of the prepared compounds, using a more biocompatible chloride abstractor, against several cancer cell lines are being studied at our laboratories, together with the possibility of engineering the dendrimers with cancer cell targeting moieties. Attempts to improve the solubility and stability of these metallodendrimers in aqueous media are also being done since the biological applications of the compounds require DMSO concentrations under 10% (v/v). The promising outcomes reported in this focus article show that low-generation metallodendrimers may be likely used as new tools in anticancer therapy. A continuous increase of interest in the field should be expected in the next years.[1]

Funding

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References

1. Rodrigues J, Jardim MG, Figueira J, Gouveia M, Tomas H, Rissanen K, “Poly(alkylidenamines) dendrimers as scaffolds for the preparation of low-generation ruthenium based metallodendrimers”, *New Journal of Chemistry* **2011**, *35*, 1938–1943.

Synthesis of new homooxacalixarene based cation and anion receptors

Ascenso J.R.[1], Paula P.M.[2]

[1]Departamento de Engenharia Química e Biológica, Centro de Química Estrutural, IST, 1049-001 Lisboa, Portugal
[2]Centro de Ciências Moleculares e Materiais, Faculdade de Ciências da Universidade de Lisboa e Faculdade de Farmácia da Universidade de Lisboa, 1649-003 Lisboa, Portugal.

Calixarene-based molecules, in particular lower rim derivatives, have been widely used in the last three decades as metal cation binders. In parallel with calixarenes development, homooxacalixarenes, that are calixarene analogues in which the CH2 bridges are partly or completely replaced by CH2OCH2 groups, have also been investigated. Among them, dihomooxacalix[4]-arene and hexahomotrioxacalix[3]arene have received significant attention as binders towards a variety of metal cations [1]. The former has a cavity size only slightly smaller than that of calix[5]arene, possesses a cone conformation and can be inherently chiral. The latter is a more flexible molecule, presents a cone conformation with C3-symmetry which can be advantageous for guests with complementary binding requirements [2].
Addition of hydrogen bond donor groups to organic hosts has been an important task to obtain recognition for specific anions. Thus, urea and thiourea binding groups have been incorporated in the calixarene scaffold to produce anion receptors. However, neutral receptors to be able to bind charged species need to overcome the tendency of the target ion to form an ion pair with its counterion, especially in low polarity organic solvents. Thus, new host molecules capable of simultaneously bind both ions of a given salt have been recently synthesised, combining the known cationic and anionic receptor motifs. Ion pair recognition by these heteroditopic receptors is an increasing interest field in supramolecular chemistry[3].
NMR spectroscopy is an extremely powerful tool in establishing the carbon skeleton and the conformation of calixarene molecules. Specifically NOESY or ROESY spectra allowed us to unequivocally prove the host to guest interations [3].

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References

1. P. M. Marcos, J. R. Ascenso, M. A. P. Segurado, P. J. Cragg, S. Michel, V. Hubscher-Bruder, F. Arnaud-Neu, “Lanthanide Cation Binding Properties of Homooxacalixarene Diethylamide Derivatives”, *Supramol. Chem.* **2011**, *23*, 93-101.
2. P. M. Marcos, J. R. Ascenso, M. A. P. Segurado, R. J. Bernardino, P. J. Cragg, Synthesis, Binding Properties and Theoretical Studies of p-tert-Butylhexahomotrioxacalix[3]arene Tri(adamantyl)ketone with Alkali, Alkaline Earth, Transition, Heavy Metal and Lanthanide Cations, *Tetrahedron* **2009**, *65*, 496-503.
3. C. Gaeta, C. Talotta, F. Farina, F. A. Teixeira, P. M. Marcos, J. R. Ascenso, P. Neri, “Alkylammonium Cation Complexation into the Narrow Cavity of
Dihomooxacalix[4]arene Macrocycle”, *J. Org. Chem*. **2012**, *77*, 10285–10293.

Metabonomics and Metabolomics

Proton high resolution magic angle spinning (HRMAS) NMR of cells in anticancer drug screening

Duarte IF[1], Lamego I[1], Marques MP[2], Gil AM[1]

[1]CICECO, Department of Chemistry, University of Aveiro, Portugal
[2]R&D Unit "Molecular Physical-Chemistry", Department of Life Sciences, Faculty of Science and Technology, University of Coimbra, Portugal

The use of cell cultures as in vitro models for studying physiological and pathological processes, as well as testing drugs and other exogenous substances, has gained refreshed interest given the emerging metabolic profiling approach based on advanced analytical tools, in particular NMR spectroscopy, and multivariate statistics.[1] Indeed, by providing a holistic view of metabolic changes and seeking consistent variation patterns triggered by certain conditions or external influences, rather than following discrete changes in individual compounds, this strategy (metabonomics) has the potential to unveil hidden biological events and allow a deeper understanding of cellular metabolism and its modulation. In our group, we have been using this approach to assess the metabolic effects induced by chemotherapy drugs on different cell lines, aiming at elucidating mechanisms of action and identifying putative toxicity/efficacy biomarkers. Following the establishment of optimised protocols for cell handling and direct analysis by ^{1}H High Resolution Magic Angle Spinning (HRMAS) NMR,[2] we have investigated the metabolic response of cultured human osteosarcoma (OS) cells (MG-63) to the drugs most commonly employed in OS chemotherapy, namely cisplatin, doxorubicin and methotrexate, known to act through distinct molecular mechanisms. The cells metabolite profiles were found to be exquisitely sensitive to culture time and drug exposure (Fig. 1). For instance, cisplatin (cis-diamminedichloroplatinum(II) or CDDP) was shown to induce significant time-dependent changes in lipids and choline-containing compounds, suggesting the occurrence of apoptosis and alterations in lipid metabolism regulation. The levels of some amino acids were also significantly altered, the decreases in glutamate and taurine possibly reflecting, respectively, effects of oxidative stress overtime and activation of cell DNA-related defence mechanisms. Moreover, significant decreases in osmoregulatory compounds myo- and scyllo-inositols were consistent with their role in cellular stress response, whereas the decrease in nitrogenated bases ado/ino possibly reflected reduced DNA synthesis. Some of these effects were common to the other drugs tested, while others, relative for example to some amino acids, seemed to be more drug-specific. Overall, this work has shown that ^{1}H HRMAS NMR of lysed cells is a powerful tool for detecting variations in a range of intracellular metabolites upon drug exposure and for unveiling dose- and time-dependent effects. The application of this approach to a potential new antineoplastic agent, palladium (Pd) spermine (sp) chelate, $(PdCl_2)_2$(sp), is currently under investigation to assess the cellular effects and mechanistic action of this promising alternative drug.

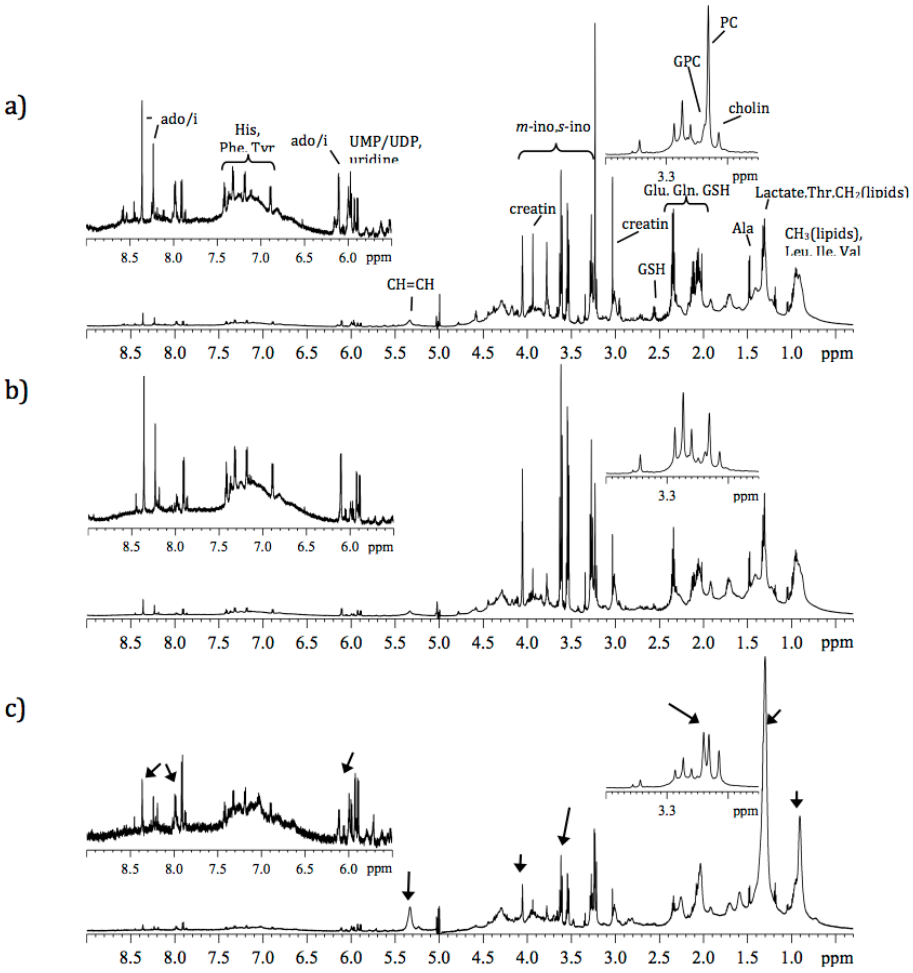

Fig. 1 – 700 MHz 1H HRMAS NMR spectra obtained for control cells at a) 0 and b) 48 hours and for c) 50 μm CDDP-treated cells at 48 hours. Arrows in c) indicate visible changes compared to controls spectrum b).

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Funding is acknowledged from the European Regional Development Fund through the Competitive Factors Thematic Operational Programme, the Foundation for Science and Technology (FCT), FEDER and POCTI. The Portuguese NMR Network supported with FCT funds is acknowledged for granting access to 500 and 800 MHz Bruker spectrometers at ITQB. We thank also CRMN- Centre de RMN à Très Hauts Champs, CNRS / ENS Lyon, France, for access to the 700 MHz NMR spectrometer and Bruker BioSpin, Germany, for providing access to spectral databases. We are grateful to the Associate Laboratory IBMC-INEB for kindly providing the MG-63 cell line.

References

[1] Duarte IF, Lamego I, Rocha C, Gil AM, "NMR metabonomics for mammalian cell metabolism studies", *Bioanalysis* **2009**, 1(9), 1597-1614.

[2] Duarte IF, Marques J, Ladeirinha AF, Rocha C, Lamego I, Calheiros R, Silva TM, Marques MPM, Melo JB, Carreira IM, Gil AM, "Analytical approaches towards successful human cell metabolome studies by NMR spectroscopy", *Analytical Chemistry* **2009**, 81, 5023-5032.

[3] Duarte IF, Lamego I, Marques J, Marques MPM, Blaise BJ, Gil AM, "A Nuclear Magnetic Resonance (NMR) study of the effect of cisplatin on the metabolic profile of MG-63 osteosarcoma cells", *Journal of Proteome Research* **2010**, 9, 5877-5886.

NMR metabonomics in disease study and diagnosis

Duarte IF[1], Barros AS[2], Goodfellow BJ[1], Gil AM[1]

CICECO[1] and QOPNA[2], Department of Chemistry, University of Aveiro, Portugal

Metabonomics entails the comprehensive analysis of endogenous metabolites within a biological system (metabolome) and the identification of metabolite patterns related to specific pathophysiological conditions or external perturbations. Among all available analytical platforms in metabonomics, NMR spectroscopy stands out as the most robust and reliable technique due to its unparalleled analytical reproducibility. Moreover, in spite of its inherently low sensitivity, high resolution ^{1}H NMR provides structural and quantitative information on a wide range of metabolites (e.g. amino acids, sugars, organic acids, nucleosides) in complex biological matrices, requiring minimal sample preparation. Our group has been applying NMR metabonomics to the investigation of different diseases, in order to characterise their metabolic signatures in tissues and biofluids and assess the corresponding potential value in disease diagnosis and follow up. Lung cancer is one of the diseases studied, in collaboration with the Faculty of Medicine and the University Hospitals of Coimbra. Tumour and non-involved adjacent tissues, collected after surgical resection and directly analysed by High Resolution Magic Angle Spinning (HRMAS) NMR, could be clearly differentiated through multivariate analysis of spectral data and putative biomarkers of malignancy were highlighted.[1] NMR metabonomics could also discriminate between lung cancer patients and healthy individuals based on blood plasma and urine metabolic profiles (Fig. 1).[2,3]

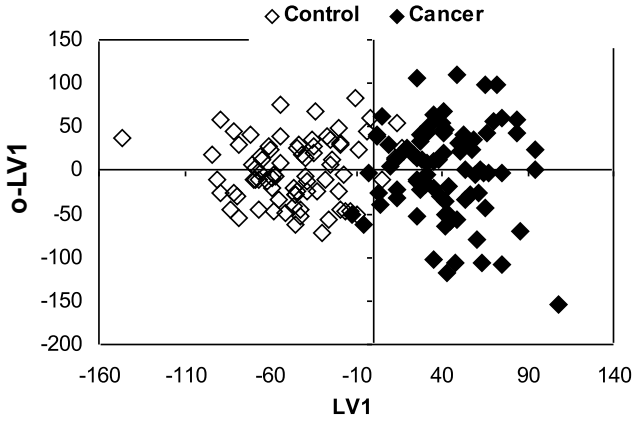
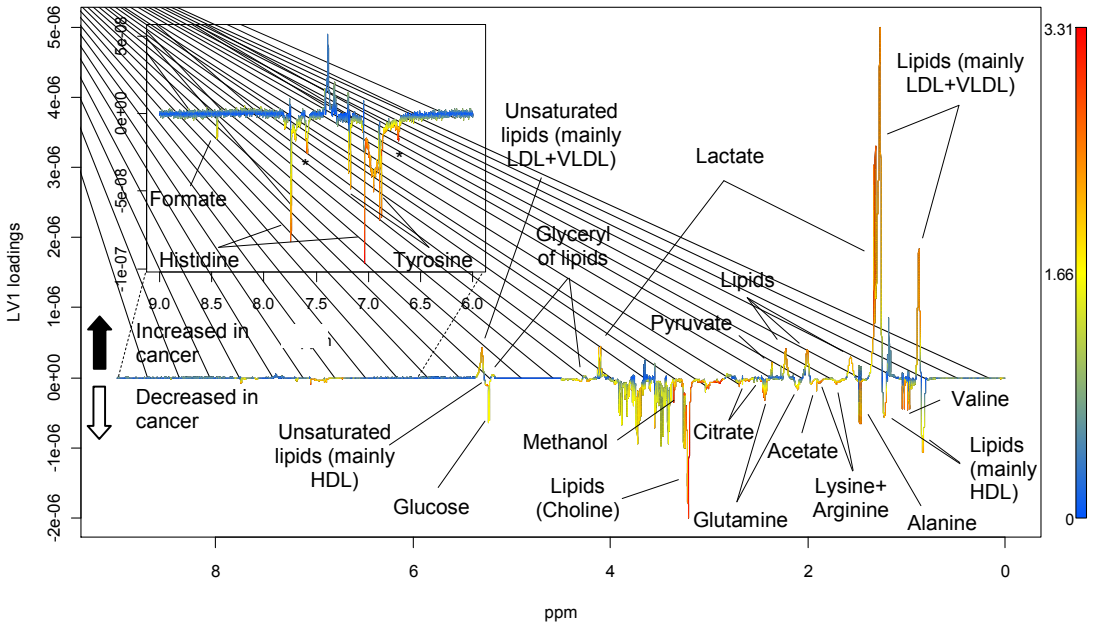


Fig. 1 - Multivariate modelling (OPLS-DA) of 500 MHz ^{1}H NMR (Carr-Purcell-Meiboom-Gill) spectra of the plasma of healthy subjects (n = 78) and lung cancer patients (n = 85): a) LV1 vs. o-LV1 scores scatter plot showing class differentiation along LV1, b) LV1 loadings plot colored as a function of Variable Importance in Projection (VIP), showing the main metabolites accounting for class differentiation (*: unassigned signals with high VIP).



In spite of the confounding influence of age and smoking status, a number of metabolites, involved for instance in glycolytic and Krebs cycle activity, were found to be consistently altered in the biofluids of patients relatively to controls. Altogether, these results show the potential of NMR metabonomics for finding putative biomarkers of lung cancer. In particular, the detection of metabolic signatures in easily accessible biofluids opens new possibilities in terms of the minimally invasive detection and monitoring of the disease. Another subject extensively investigated by our group, in collaboration with Bissaya Barreto Maternity and the Faculty of Medicine of Coimbra, is the search for metabolic markers of pregnancy disorders, through NMR metabonomics of amniotic fluid (AF) and maternal urine and blood plasma[4-6]. Among the disorders studied, foetal malformations were found to have the highest impact on the composition of all biofluids. In particular, changes in AF pointed to altered energy metabolism and kidney underdevelopment in malformed foetuses, together with additional effects on protein and nucleotide biosynthesis. Several metabolites were also found to be consistently altered in maternal plasma and urine, unveiling perturbations in several metabolic pathways and suggesting a systemic signature for foetal malformations. Pre-diagnosed gestational diabetes was also found to induce detectable metabolic changes in the biofluids studied, especially in AF and urine, while chromosomal disorders could be differentiated from healthy pregnancies mainly based on maternal urine composition. This approach is currently being extended to the analysis of newborn urine to attempt correlation between other prenatal disorders such as preterm delivery and newborn health.

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References

[1] Rocha C, Barros AS, Gil AM, Goodfellow BJ, Humpfer E, Spraul M, Carreira IM, Melo JB, Bernardo J, Gomes A, Sousa V, Carvalho L, Duarte IF, "Metabolic profiling of human lung cancer tissue by ^{1}H High Resolution Magic Angle Spinning (HRMAS) NMR spectroscopy", *Journal of Proteome Research* **2010**, 9, 319-332.
[2] Carrola J, Rocha CM, Barros AS, Gil AM, Goodfellow BJ, Carreira IM, Bernardo J, Gomes A, Sousa V, Carvalho L, Duarte IF, "Metabolic signatures of lung cancer in biofluids: NMR-based metabonomics of urine", *Journal of Proteome Research* **2011**, 10, 221-230.
[3] Rocha CM, Carrola J, Barros AS, Gil AM, Goodfellow BJ, Carreira IM, Bernardo J, Gomes A, Sousa V, Carvalho L, Duarte IF. "Metabolic signatures of lung cancer in biofluids: NMR-based metabonomics of blood plasma", *Journal of Proteome Research* **2011**, 10, 4314-4324.
[4] Graça G, Duarte IF, Barros AS, Goodfellow BJ, Diaz S, Pinto J, Carreira IM, Galhano E, Pita C, Gil AM, "The impact of prenatal disorders on the metabolic profile of 2nd trimester amniotic fluid: a Nuclear Magnetic Resonance (NMR) metabonomic study", *Journal of Proteome Research* **2010**, 9, 6016–6024.
[5] Diaz SO, Pinto J, Graça G, Duarte IF, Barros AS, Galhano E, Pita C, Almeida MC, Goodfellow BJ, Carreira IM, Gil AM, "Metabolic biomarkers of prenatal disorders: an exploratory NMR metabonomics study of 2nd trimester maternal urine and blood plasma", *Journal of Proteome Research* **2011**, 10, 3732-3742.
[6] Graça G, Goodfellow BJ, Barros AS, Diaz S, Duarte IF, Spagou K, Veselkov K, Want EJ, Lindon JC, Carreira IM, Galhano E, Pita C, Gil AM, "UPLC-MS Metabolic Profiling of Second Trimester Amniotic Fluid and Maternal Urine and Comparison with NMR Spectral Profiling for the Identification of Pregnancy Disorder Biomarkers", *Molecular BioSystems* **2012** DOI: 10.1039/c2mb05424h.

Metabolic analysis of the acid stress response in *Lactococcus lactis*: a basis for the development of acid resistant strains

Ana Lúcia Carvalho[1], David L. Turner[1], Luís L. Fonseca[1], Ana Solopova[2], Teresa Catarino[1], Oscar P. Kuipers[2], Eberhard O. Voit[3], Ana Rute Neves[1], and Helena Santos[1]

[1]Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Av. da República – EAN, 2780-157 Oeiras, Portugal.
[2]Department of Molecular Genetics, Groningen Biomolecular Sciences and Biotechnology Institute, University of Groningen, P.O. Box 14, 9750 AA, Haren, the Netherlands.
[3]Integrative BioSystems Institute and The Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, Atlanta, Georgia, United States of America.

Lactococcus lactis is a mesophilic Gram-positive bacterium of great economical value due to its worldwide application in a variety of dairy fermentations. Despite its contribution to the organoleptic and nutritional properties of the fermented products, *L. lactis* is better known for its ability to provide effective means of food preservation. This lactococcal trait derives directly from its simple metabolism, in which sugars are converted into lactic acid and energy is conserved mainly through substrate level phosphorylation. As a consequence of lactic acid production the pH of the medium drops leading to decreased glycolytic flux and growth rate, and ultimately compromising cell viability (van de Guchte *et al.*, 2002). In this study the effect of pH on glucose metabolism of non-growing cells of *L. lactis* MG1363 was studied in a non-invasive manner by NMR in the range of 4.8 to 6.5. Time series were obtained by ^{13}CNMR for glucose consumption, glycolytic intermediates and end-product accumulation (Neves *et al.*, 1999). Immediate pH effects on glucose transporters and/or metabolic enzyme activities were distinguished from transcriptional/translational effects by careful design of the experimental conditions. Hence, glucose metabolism was investigated at different values of external pH (controlled at 6.5, 5.5, 5.1 and 4.8) in *L. lactis* grown at optimal pH of 6.5 to assess direct effects of acidic pH on metabolism; in addition, cells grown at pH 5.1, were used to assess the level of transcriptional adjustment to low pH. In cell suspensions that had been grown at optimal pH, the glucose consumption rate decreased progressively with the increase in the extracellular proton concentration. Importantly, the different pH values of the intracellular and extracellular compartments, and consequently the disparate degree of lactic acid dissociation, led to distinct NMR resonances arising from the intracellular and extracellular pools of this organic acid (Fig. 1.).

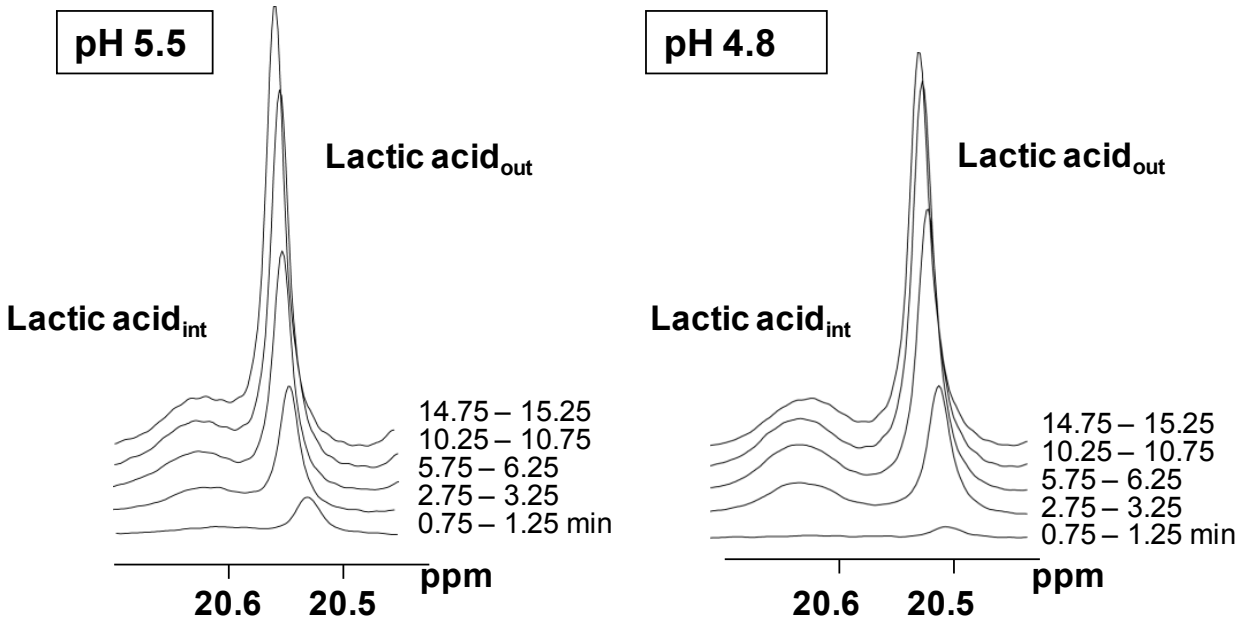

Fig. 1. Sequences of ^{13}C-NMR spectra obtained during glucose metabolism at external pH values of 5.5, and 4.8, showing two resonances, assigned as intracellular and extracellular lactic acid.

L. lactis remained homolactic independently of the medium pH, and at sub-optimal pHs, the intracellular lactic acid reached approx. 450 mM irrespectively of the pH examined. Cells grown at pH 5.1, and thus adjusted to acidic conditions, showed a metabolic performance superior to that of cells grown at optimal conditions and challenged with identi-

cal pH conditions (Fig 2.). Glucose metabolism at pH 5.1 proceeded at a rate that was 50% higher, whereas the maximal intracellular lactate concentration reached considerably higher values, *i. e.*, 700 mM, thus generating a lactate gradient that surpassed by far the proton gradient barrier.
In view of these results, the development of a *L. lactis* strain with improved acid resistance should consider the following guidelines: overexpression of the H^+-ATPase activity, glucose transporters (PTS^{Cel} and PTS^{Man}) and the glycolytic enzymes phosphofructokinase, pyruvate kinase and lactate dehydrogenase.

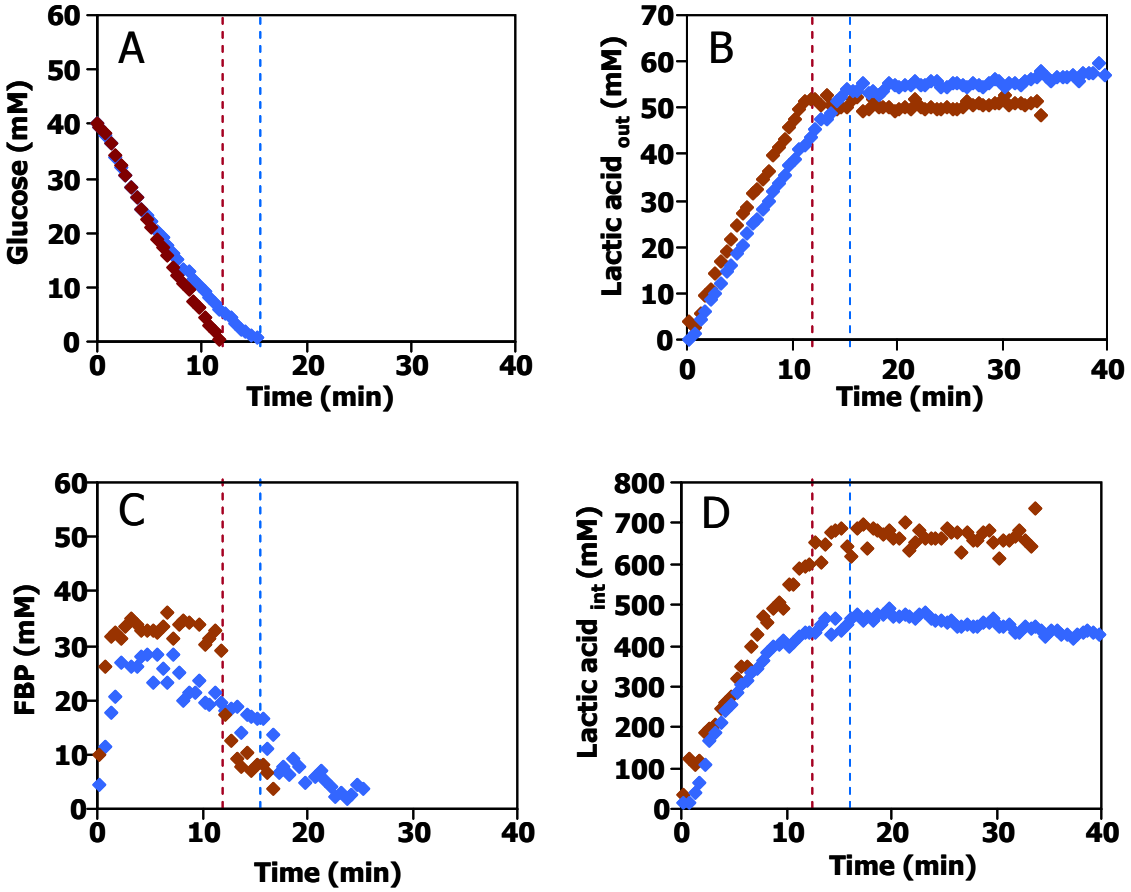

Fig. 2. Metabolite time series obtained during glucose metabolism in non-growing cells of *L. lactis* MG1363 grown at 6.5 (blue diamonds) or 5.1 (brown diamonds). The metabolite pools were monitored online by *in vivo* ^{13}CNMR at 30 ºC, under anaerobic conditions and pH controlled at 5.1. A) Kinetics of [1-^{13}C]glucose (40 mM) consumption, B) extracellular lactic acid formation, C) pools of fructose 1,6-bisphosphate, and D) profiles of intracellular lactic acid. Each experiment was performed twice with good reproducibility.

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References

Neves, A.R., Ramos, A., Nunes, M.C., Kleerebezem, M., Hugenholtz, J., de Vos, W.M. Almeida, J., and Santos, H. (1999) *In vivo* nuclear magnetic resonance studies of glycolytic kinetics in *Lactococcus lactis*. *Biotechnol Bioeng* **64**:200-212.
van de Guchte, G.M., Serror, P., Chervaux, C., Smokvina, T., Ehrlich, S.D., and Maguin, E. (2002) Stress responses in lactic acid bacteria. *Antonie Van Leeuwenhoek* **82**:187-216.

In vivo MR studies to validate the promising anti-diabetic and anti-obesity capacity of a new vanadium compound

A. M. Metelo[1], R. Pérez – Carro[2], P. López – Larrubia[2] and M. M. C. A. Castro[1]

[1] Department of Life Sciences, Faculty of Science and Technology, and Center of Neurosciences and Cell Biology, University of Coimbra, Portugal
[2] Instituto Investigaciones Biomedicas Alberto Sols, CSIC, Universidad Autonoma de Madrid, Madrid, Spain

Diabetes *mellitus* (DM) is the world's fastest-growing disease being responsible for almost 3 million deaths worldwide per year [1]. In recent years, vanadium compounds have attracted a lot of interest due to their potential therapeutic application, particularly in the treatment of DM [2]. Many V(IV) and V(V) complexes have been synthesized, in a search for desired properties such as hydrolytic stability, water solubility, neutral charge and/or lipophilicity, and their toxicity and insulin mimetic action have been evaluated. In this work we report an *in vivo* study with Zucker fatty (fa/fa) rats treated during four weeks with the compound $V^{IV}O(dmpp)_2$ (Fig. 1), which has shown promising insulin-mimetic properties through *ex vivo* studies with rat adipocytes [3]. Gain of body weight was daily determined and glucose tolerance test was performed at the end of the study. Hepatic and subcutaneous lipid content were assessed by Magnetic Resonance Imaging (MRI) and Spectroscopy (MRS). The obtained results show that gain of body weight, hepatic triglycerides conten and subcutaneous fat width of obese-treated Zucker rats were significantly lower than that of obese non-treated Zucker rats, indicating a specific biological activity of $V^{IV}O(dmpp)_2$ in mitigating impaired lipid metabolism. In addition, the typical glucose intolerance profile of fatty rats was reversed by the action of $V^{IV}O(dmpp)_2$. All these results corroborate previous data obtained with *ex vivo* experiments [3], and demonstrate the insulin-mimetic capacity of $V^{IV}O(dmpp)_2$ in Zucker fatty rats, a pre-diabetic animal model [4].

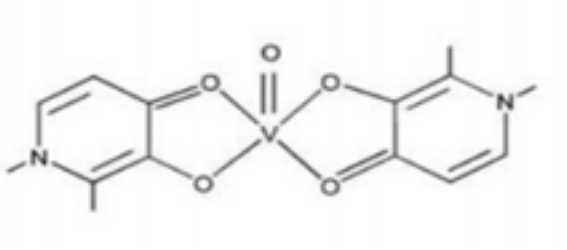


Figure 1- Schematic representation of the molecular structure of the V(IV) complex $V^{IV}O(dmpp)_2$ - bis-[3-hydroxy-1,2-dimethyl-4-pyridinonate] oxovanadium (IV).

References

[1] Wild S *et al*. *Diabetes Care*. 2004, 27(5):1047-1053.
[2] Thompson K *et al*. *Journal of Inorganic Biochemistry*. 2009, 103(4):554-558.
[3] Passadouro M *et al*. *Journal of Inorganic Biochemistry*. 2010, 104(9):987-992.
[4] Augstein P & Salzsieder E. *Methods in Molecular Biolog.* 2009, 560:159-189.

Papilio machaon pupa follow-up by MR Micro-imaging

Alexandra Carvalho[a], G. Feio[a], Pedro Almeida[a], M. João Verdasca[b], Miguel A. Reis[c]

a) CENIMAT/I3N – Faculdade de Ciências e Tecnologia - UNL, Campus da FCT, Quinta da Torre 2825 - 114 Caparica, Portugal
b) Lagartagis, Museu Nacional de História Natural, Rua da Escola Politécnica, 581250-102 Lisboa, Portugalc) Campus Tecnológico e Nuclear IST/ITN, Estrada Nacional 10, 2686-953 Sacavém – Portugal

The follow-up of a *Papilio machaon* pupa metamorphosis has been studied by Magnetic Resonance Micro-imaging. The *Papilio machaon* is a beautiful butterfly of the Papilionidae family, with two to three broods in a year, existing in Europe, Asia and North America. The pupa of this specie is attached upright to a plant stem by a silk girdle. It exhibits a distinct colour polymorphism, being principally green and yellow, or brown, and white. Not much is known about the metamorphosis details of this Lepidoptera, in particular regarding the wings development. The wings structure is our main interest in this study because these lepidoptera wings are made of natural photonic crystal materials which are attracting a lot of attention for both fundamental and technological reasons [1]. In our study we have obtained a series of images of the pupa in a four week interval with an image collection on a twice a week basis.

A multinuclear nuclear magnetic resonance spectrometer, Bruker Avance III, operating at 7 T, equipped with a micro-imaging probe and a 60A XYZ pulsed gradients system, was used to obtain a set of sagittal slices with a 0.25 mm thickness and 0.75 mm inter-slice distance, with a multi-slice multi-echo protocol optimized with TE=4.594 ms, TR=707.668 ms with a 256 matrix of 6x6 μm2 pixels and 8 excitations. The sample was ventilated in order to keep the temperature compatible with the lepidoptera development environment.

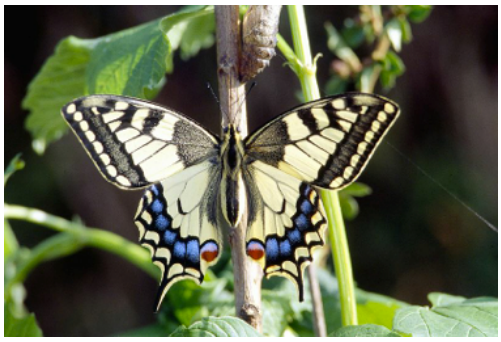


Fig. 1: An adult *Papilio machaon*

A set of images is presented in Fig. 2, which we believe to be the first of a *Papilio machaon* pupa, in different stages of metamorphosis and should therefore contribute to through some light in the wings development process.
Photonic crystals (PC) are optical nanostrutures that affect the movement of photons in a same way a semiconductor crystal affects the electrons movement [1].
Apart from being beautiful natural, PC also have various patterns that are quite promising structural matrices for creating novel optical devices

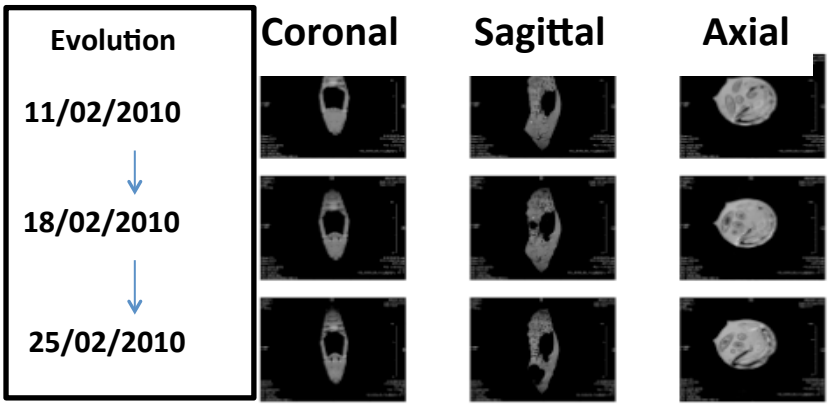


Fig. 2: Follow-up of a *Papilio machaon* pupa metamorphosis by Magnetic Resonance Micro-imaging.

Funding: Portuguese Nuclear Magnetic Resonance Network (PTNMR).

References:

[1] J. D. Joannopoulos, S.G. Johnson, J. N. Winn, R. D. Meade, Photonic Crystals Molding the Flow of Light, Second Edition, Princeton Uni. Press, (2008)

New long circulating magnetoliposomes as negative contrast agents for MRI

M.B.F. Martins[1],M. L. Corvo[1], P. Marcelino[2], F. Fontes[3], H.S. Marinho[3], G. Feio[4], A.Carvalho[4]

[1]iMed/FF/UL, Av. Prof. Gama Pinto, 1649-003 Lisboa, Portugal
[2]CEDOC/ FCM/ UNL, Campo dos Mártires da Pátria, 1169-056 Lisboa, Portugal
[3]DQB & CQB, FC/UL, Campo Grande, 1749-016 Lisboa, Portugal
[4]CENIMAT-I3N/DCM/FCT/UNL, Campus da Caparica, 2829-516 Caparica, Portugal

For a long time liposomes and in particular magnetoliposomes have been used in medicine due to their remarkable properties, namely: a) high biocompatibility, b) possibility of several surface manipulations, c) possibility to enclose both hydrophilic as well as hydrophobic compounds, d) ability to simultaneously contain imaging and therapeutic agents and c) controllable size, from 20 nm to 1 μm with a relatively high degree of accuracy. In this work the potentiality, as a negative contrast agent for MRI, of a new long circulating liposoma formulation, loaded with 10 nm iron oxide nanoparticles which have been coated with polyethylene glycol (PEG), was investigated. The encapsulation parameters obtained and the size of the loaded liposomes make this system a good tool to be used as a negative contrast agent to visualize inflammatory sites after ischemia-reperfusion injuries. The described magnetoliposomes were tested in a rat model of liver ischemia, performed after hepatic artery and porta vein occlusion. The relaxivities r_1, r_2 and r_2^*, were obtained in a Bruker AVANCE III spectrometer in a magnetic field of 7 T (300 MHz for proton), a very interesting value for the clinical applications. MRI images, at 7 T, were obtained for rat liver after 30 min of partial ischemia and 24h of post-treatment with and without the developed magnetoliposomes, and the contrast enhancement measured.

The long circulating nanosystem developed by us had a minor effect on T_1 , but a strong one for T_2 and mainly on T_2^*. Therefore the results obtained by this preliminary study indicate that this nanosystem may be a potential negative contrast agent.

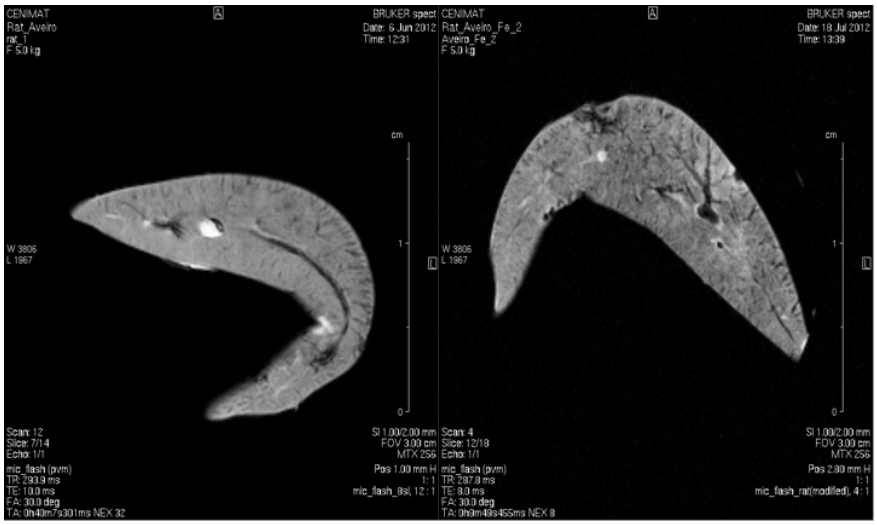


Fig.1: Magnetic resonance microimaging of: rat liver after 30 min of partial ischemia (left), rat liver after 30 min of partial ischemia and with the developed magnetoliposomes (right), obtained at a 7 T magnetic field and with a gradient field of 160G/cm.

Funding
PEst-OE/QUI/UI0612/2011, Pest-OE/SAU/UI4013/2011, Sociedade Portuguesa de Transplantação - Bolsa de Investigação SPT/ Astellas; Strategic Project Pest-C/CTM/LA0025/2011; Portuguese Nuclear Magnetic Resonance Network (PTNMR)

References

M.B.F. Martins,M. L. Corvo, P. Marcelino, H.S. Marinho, G. Feio, A.Carvalho, "New long circulating magnetoliposomes as negative contrast agents for MRI" submitted to *Nanomedicine, Nanotechnology,Biology and Medicine*.
Carvalho A., Gonçalves M. Clara, Martins M. B., Meixedo D., Feio G.,"Relaxivities of Magnetoliposomes: the effect of cholesterol", *Magnetic Resonance Imaging* in press.

Potentiality of ORMOSIL nanoparticles as negative Contrast Agents for MRI

M.C. Gonçalves[1], L. Fortes[1], G. Feio[2], A.Carvalho[2]

[1]Dep. Chemical Eng., IST, UTL, Av. Rovisco Pais, 1049-001 Lisboa, Portugal, and ICEMS, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
[2]CENIMAT-I3N/DCM/FCT/UNL, Campus da Caparica, 2829-516 Caparica, Portugal

We have studied a new application of Ormosil as contrast enhancement agents for magnetic resonance imaging [1], when coating iron oxide nanoparticles. The introduction of various organic functional groups, by a judicious choice of the ratio of hydrophilic (e.g. vinyl-) to hydrophobic (e.g. methyl-) monomers during the sol-gel synthesis of silica has led to organically modified silica, known as ORMOSIL. For long that these materials are use in nanomedice mainly for gene or drug deliver. Some applications in other imaging modalities, as fluorescence, have been reported, but as far as we know, as negative contrast agent for IRM, this is a new approach. We measured the relaxivities r_1, r_2 and r_2^* for different Ormosil and silica [2] with a superparamagnetic core of Iron Oxide nanoparticles of 6nm diameter (Fig. 1). The measurement of the longitudinal and transversal relaxation times was obtained in a Bruker AVANCE III spectrometer in a magnetic field of 7 T (300 MHz for proton). The preliminary results allows to say that the Ormosil effect on T_1 is minor, but on T_2, and more effectively on T_2^*, a strong effect has been observed. This is the expected behaviour of a good negative contrast agent.

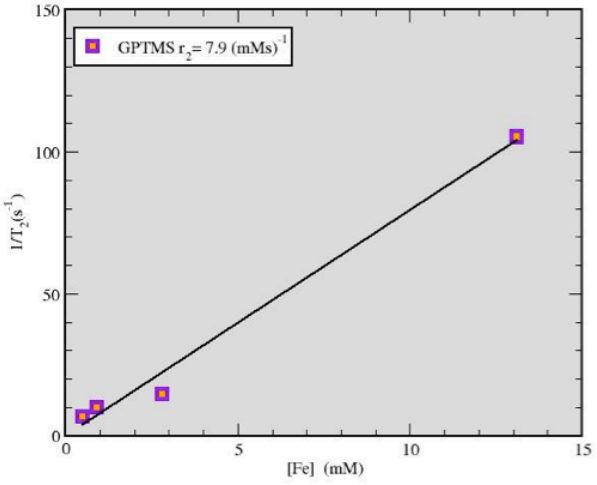


Fig.1: Transverse relaxation rate for a ORMOSIL core shell

Funding

PEst-OE/QUI/UI0612/2011, Pest-OE/SAU/UI4013/2011, Sociedade Portuguesa de Transplantação - Bolsa de Investigação SPT/ Astellas; Strategic Project Pest-C/CTM/LA0025/2011; Portuguese Nuclear Magnetic Resonance Network (PTNMR)

References

[1] A. Carvalho, M. Clara Gonçalves, R. Colaço, G. Feio,"Ormosil superparamagnetic nanoparticles as negative contrast agents for MRI", submitted to Nanoscale Research Letters.

[2] C. Huanga, K. G. Neoha , L.Wanga, E. Kanga and B. Shuter, Contrast Med.Mol. Imaging, 6, 298-307, (2011)

Activity Indicators

To better evaluate the impact of the National NMR Network in the national scientific panorama the following indicators were selected:

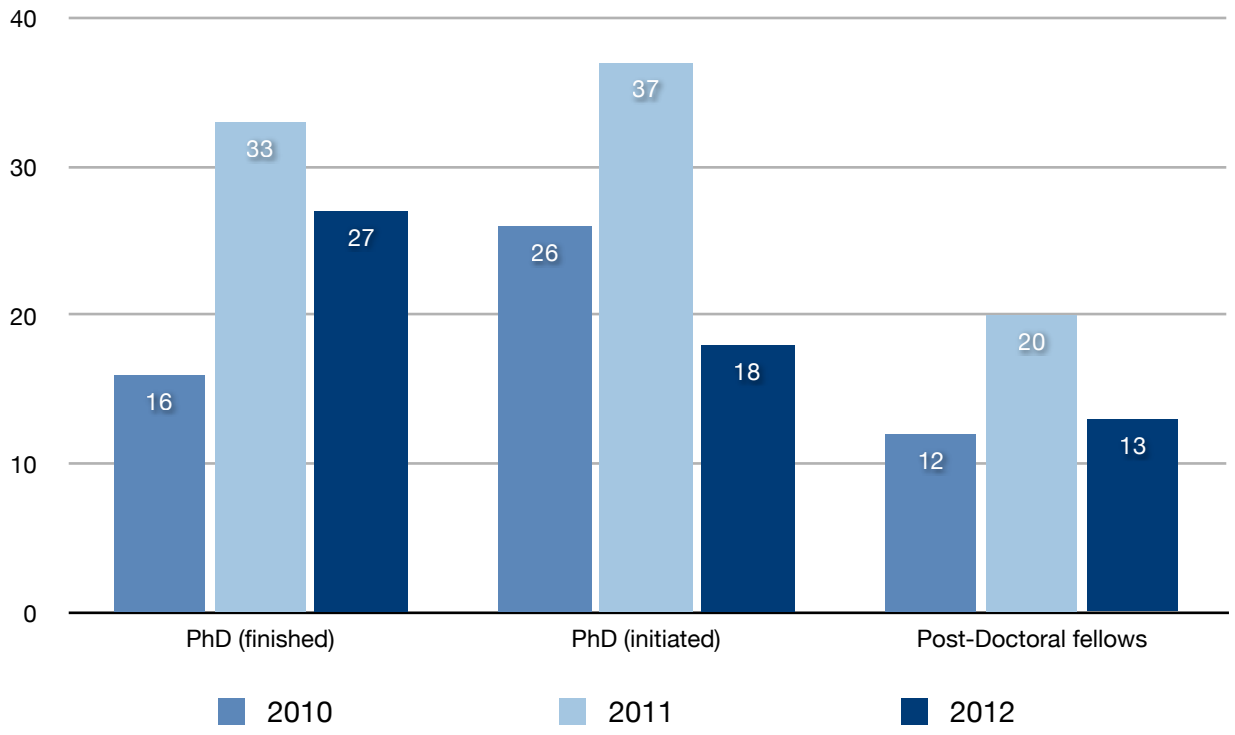
Advanced training - the number of PhD thesis started and completed in each year as well as the number of Post-Doc researchers initiating NMR related work in each year;

Research projects - the number of research projects and grants approved in 2010-2012;

Publications - the number of publications in peer reviewed journals in each year.

Only grants and projects where NMR was used strictly as a main tool were considered, as well as publications whose work was clearly supported by the PTNMR infrastructure. Figure 3, resumes the advanced training indicators with a comparison for the years 2010 - 2012.

Figure 3 – Advanced training of human resources 2010-2012

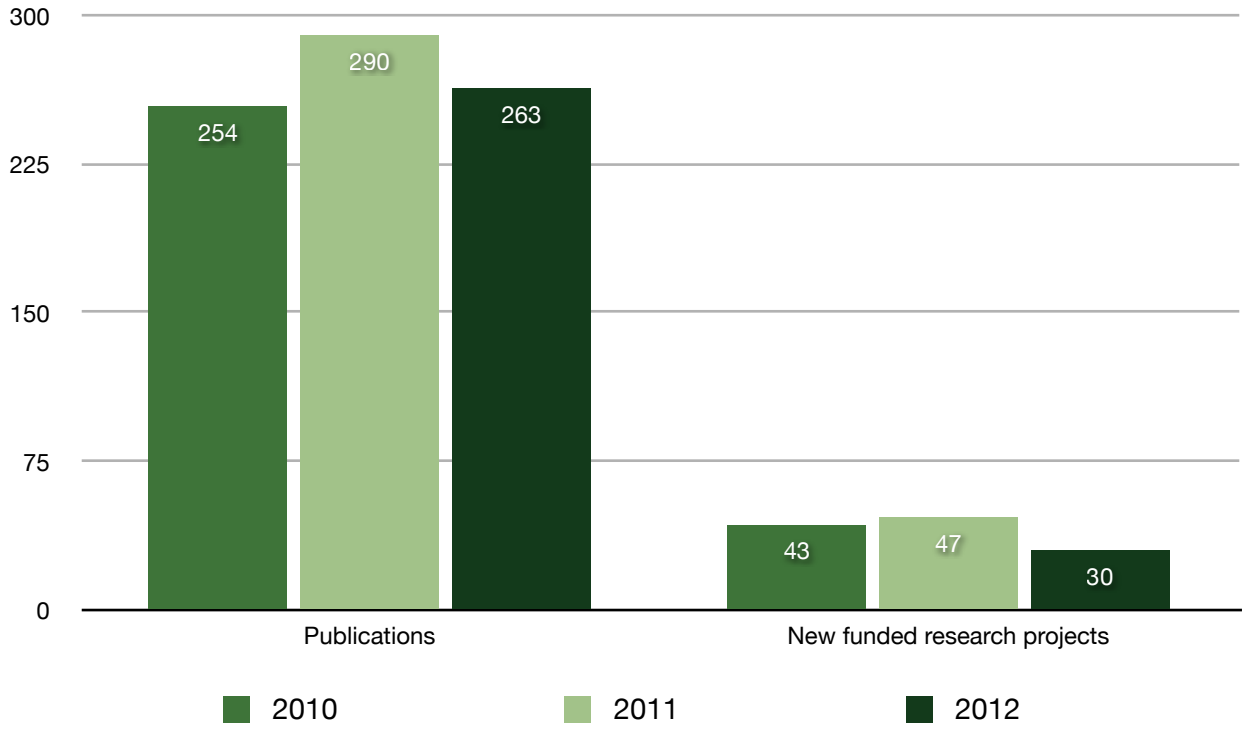


The numbers in figure 3 clearly demonstrate the importance of the PTNMR network in supporting advanced scientific training and research. The numbers relative to 2012 show a great reduction (close to 50 %) of new PhDs and Post-doctoral fellows when compared to 2011. While this is a substantial decrease it reflects the number of grants available through the annual competition promoted by FCT-MEC and cannot be interpreted as a decrease in the support of the network to the advanced training.

The impact of the PTNMR network in human resources training goes beyond the numbers expressed in figure 3 since it is equally important to take into account the number of Master students (MSc.) and young undergraduate students engaged in scientific research projects supported by the infrastructure (data not compiled). For all those, NMR techniques are imperative on their curriculum and research plans.

To characterize in more detail the impact of the PTNMR network in the scientific production the number of publications in peer reviewed journals and the number of new funded research projects in 2010- 2012 were compiled (figure 4). This last indicator allows to evaluate the contribution of the National NMR Network to the competitiveness in getting funds through research projects. For a rigorous analysis only those projects were NMR is used systematically in the research plans were considered.

Figure 4 – Publications and New Funded Research Projects 2010-2012



From figure 4, the average number of published papers in peer reviewed journals, 269, and the average number of new approved research projects, 40, were determined. A full list of the publications organized by PTNMR Unit can be found in annex 2, a full list of supported research projects is presented in annex 3.

These numbers clearly demonstrate the contribution of the PTNMR network to the national scientific community in terms of scientific production as well as to the competitiveness of the research proposals.

Annex 1

PTNMR Management Rules and User Policies

These user policies are subject to revision and updates. Consult the website http://ptnmr.dq.ua.pt for the most recent version. Please forward your comments and suggestions to the Network Coordinator or to the heads of each NMR unit.

Duties

The PTNMR network is a national scientific hub funded by the Portuguese Foundation for Science and Technology (FCT-MEC). With the support of more than nine Portuguese Universities and Institutions, the Network has been created to provide Portuguese researchers access to state-of-the-art NMR equipment nationwide. The PTNMR Network is intended to support research projects, the scientific Portuguese research community and provide services to companies and industry.

Management

The PTNMR network is organized and managed according to a policy agreed between all NMR partners (NMR units) and the Portuguese Foundation for Science and Technology (FCT-MEC). All documents are freely available on http://ptnmr.dq.ua.pt according to the transparency policy defined with FCT-MEC. This document establishes the network mission and management, the type of services offered to the community, the rules and conditions for access to the network services and the duties and responsibilities of the users and the network institutions.

The management structure of the PTNMR network consists of an International Advisory Board, a Management Committee headed by a General Coordinator, and a Manager per unit.

The International Advisory Board

The International Advisory Board consists of three members, recognized experts of the international NMR community. The members are appointed by the Management Committee. The duty of the Management Committee is to review the Annual Report of the operations of the PTNMR Network, and provide comments, suggestions and recommendations on the efficiency of the operations, on the basis of the evaluation of the report.

International Advisory Board:
Prof. Christian Griesinger (MPI - Goettingen)
Prof. Hans Wolfgang Spiess (MPI - Mainz)
Prof. Lucia Banci (CERM - Florence)

The Management Committee

Is responsible to approve the annual financial budget and is responsible for the operational of all PTNMR network. Their main responsibility is to coordinate the development of all NMR units keeping in mind the high levels of services offer to all Portuguese scientific community, and takes actions to implement the necessary improvements. Its mandate consists also of establishing the rules for access to the Network and improving the general operations for a cost effective network. The Management Committee reviews periodically the structure of user fees, the budget of each NMR unit, the proposed courses/seminars/conferences and submits reports to be compiled onto the Annual Report of the PTNMR network.

Management Committee (2010 - 2012):
Assis Farinha Martins (FCT-UNL)
Baltazar Castro (Universidade do Porto)
Carlos Geraldes (Universidade de Coimbra)
Carlos Romão (ITQB-UNL)
Eurico J. Cabrita (FCT-UNL) - General Coordinator 2010-2012
João Rocha (Universidade de Aveiro)
João Rodrigues (Universidade da Madeira)
José do Rosário Ascenso (IST-UTL)
Maria João Queiroz (Universidade do Minho)
Helena Santos (ITQB-UNL)

NMR Unit Manager

The NMR manager is responsible for the day-to-day operations. The manager is the liaison between the users and the Management Committee providing assistance and support to all users. The unit manager is responsible for the time allocation in the spectrometers (directly or under recommendation of the Project Evaluation Panel) and for the training of the users. It is also the duty of the NMR unit manager to maintain a dedicated webpage of the Unit including a public updated calendar of spectrometer use and a list of equipment and services and to submit reports and publications to the Main Coordinator to help ensure the continuity of services and the Network. All information will be compiled at the end of the year and included in the Annual Report prepared by the Network Coordinator.

Project Evaluation Panel

Is responsible for the evaluation of project proposals for spectrometer use. Evaluates the proposals concerning scientific merit and adequacy of requested NMR time. The Management board is responsible for the designation of the specialists in the panel.

PTNMR Network Guidelines

Users are encouraged to operate the instruments on their own after authorisation by the NMR unit manager of the local NMR affiliated centre. It is expected that each person who is approved to be a NMR user will have, at the minimum: prior experience on a modern NMR instrument, either through outside NMR activities or hands-on training courses. All users should be familiarised themselves with the NMR equipment and though technique to guarantee not only its safety and durability but also its rentability in terms of time. Scientific data must be recognised as having a potential value that may exceed publications immediately derived from it. It is mandatory for the PTNMR network and all affiliated centres to provide adequate quality assurance to satisfy funding bodies of our ability to deliver the promised scientific results.

Users are responsible for damage that results from samples that are explosive, pressurized, chemically corrosive, radioactive, biologically dangerous, or that otherwise pose unusual hazards to instrumentation or personnel. In all such cases, prior permission and advice should be sought with regard to these special samples, but permission does not absolve any user from responsibility for whatever harm their samples may cause on any spectrometer or probe from the PTNMR network. Users using PTNMR resources showing misbehaviour or negligent use of the NMR equipment may be held responsible for their acts. This obligation does not extend to responsibility for damage that occurs accidentally and unavoidably during normal use. Any possible damage must immediately be reported to the NMR manager.

Spectrometer Use

Spectrometer use is managed by the Unit manager according to three types of use:
- regular (direct decision by the Unit manager)
- project based (by recommendation of the Project Evaluators Panel)
- service to companies

Time management and allocation to users depends on the category of Spectrometer. PTNMR spectrometers are divided into two categories according to the Magnetic Field:

High Field Spectrometers (above 600 MHz)
Spectrometer use is managed in a monthly base with the following priority rules:
- 70 % of the total spectrometer available to external users

Low Field Spectrometers (below 600 MHz)
Spectrometer use is managed in a weekly base with the following general rules:
- 30 % of the total spectrometer time available to external users

Each Unit Manager is responsible for publishing the general rules for spectrometer use and the forms for project proposals in their unit webpage. Project Proposals are send by the Unit Manager to the General Coordinator. The General Coordinator forwards the proposal to 2 specialists from the Project Evaluators Panel. The decision should be communicated to the Unit Manager and the User in no more than a week after receiving the proposal.

User fees
The rates for accessing the NMR equipment belonging to the PTNMR network are estimated according to the instructions indicated below and are available upon request.

The full cost of running a spectrometer belonging to the PTNMR network covers the cryogens and other consumables, service contracts and repairs, NMR staff time dedicated to running the facility, building charges and depreciation of some equipment. Thus, user price for each spectrometer must be calculated according to the NMR equipment basis on the annual running costs. The total cost will be updated for researchers and investigators according to the external funding provided from FCT-MEC, the main sponsored of the PTNMR network.

Equation 1 shows the user cost time:

User Cost per hour = [Financial Support from FCT/MEC – (Maintenance + personnel cost)] / 8760 hours

In which Maintenance is calculated according to:

Maintenance = gases + annual NMR maintenance contract + repairing's not included on the annual maintenance contract

Note: the user cost applied on Equation 1 implies the use of the total time per annum and not the real user NMR time. This may imply if the total user NMR time is shorter than the total annual time the research unit/institution hosting the spectrometer must cover the extra cost. Academic users should be aware that in economic stringency from the main funding body FCT-MEC, funds may be cut and though researchers are expected to contribute to some of the critical costs associated with operating the facility. However, it should be understood that the stated academic access fees cover only a fraction of the total costs of operation.

The PTNMR network was principally established to support peer reviewed academic research in Portugal through generous funding from FCT-MCE. Therefore, external users outside I&D sponsored by FCT-MCE are not supported by the Network. Prices are established by each NMR unit guaranteeing the fairness competition rules of the market.

Travel Support
The PTNMR Network has a policy of sponsoring travel and accommodation expenses for Portuguese academia with manifested interest in using NMR in their main research activities. All requests should be submitted by a supervisor in

advance (one month earlier) of the trip. Requests should be forwarded to the managers of the following NMR centres: ITQB-UNL, REQUIMTE-FCT-UNL and CNC-Univ. Coimbra, for review and approval by the head of the NMR unit.

Annual Progress Report

Each year the PTNMR network has the obligation to release an annual report stating all information concerning the scientific, financial and operational activities concerning all NMR partners. Following this directive will ensure that the instrumentation time is allocated properly for scientific national research not compromising external services to industry.

The reports are freely available on the main web server of the Network (ptnmr.dq.ua.pt) allowing a public surveillance of the activities performed by the PTNMR. The reports should state the public spending on the PTNMR network and the accomplished tasks proposed per year by the management committee. The adequate reporting is vital in securing continuing financial support of the PTNMR operations by the funding agency (FCT-MEC). Cooperation of our users in this matter is therefore appreciated.

Acknowledgments

All users are required to acknowledge use of PTNMR network in any scientific publications and communications that benefit from its services with the following statement:

We acknowledge the Portuguese National NMR Network (RNRMN), supported with funds from Fundação para a Ciência e a Tecnologia (FCT).

Annex 2

Publications in 2010 - 2012

CENIMAT – FCT – Universidade Nova de Lisboa

Scientific Papers

Godinho MH, Canejo JP, Feio G, Terentjev EM "Self-winding of helices in plant tendrils and cellulose liquid crystal fibers" Soft Matter, 6, 5965-5970 (2010). http://dx.doi.org/10.1039/C0SM00427H

Figueirinhas JL, Feio G, Cruz C, Lehmann M, Kohn C, Dong RY "Nuclear magnetic resonance spectroscopic investigations of phase biaxiality in the nematic glass of a shape-persistent V-shaped mesogen", J. Chem. Phys., 133 174509 (2010). http://dx.doi.org/10.1063/1.3496491

Kundu S, Feio G, Pinto LFV, Almeida PL, Figueirinhas JL, Godinho MH "Deuterium NMR Study of Orientational Order in Cellulosic Network Microfibers" Macromolecules, 43 (13): 5749-5755 (2010). http://dx.doi.org/10.1021/ma100882w

Lehmann M, Kohn C, Figueirinhas JL, Feio G, Cruz C, Dong RY "Biaxial Nematic Mesophases from Shape-Persistent Mesogens with a Fluorenone Bending Unit" Chemistry 16 (28): 8275-8279 (2010). http://dx.doi.org/10.1002/chem.201001214

Martins AF, Veron A "Theory and numerical simulation of field-induced director dynamics in confined nematics investigated by nuclear magnetic resonance" Liquid Crystals, 37 (6-7): 747-771 (2010). http://dx.doi.org/10.1080/02678292.2010.485837

Carvalho A, Goncalves MC, Martins MB, Meixedo D, Feio G. "Relaxivities of magnetoliposomes: The effect of cholesterol" Magn Reson Imaging., [Epub ahead of print] (2013). http://dx.doi.org/10.1016/j.mri.2012.10.024

CERMAX - ITQB - Universidade Nova de Lisboa

Book Chapters

H. Santos, P. Lamosa, N. Borges, L. G. Gonçalves, T. M. Pais & M. V. Rodrigues "Organic Compatible Solutes of Prokaryotes That Thrive In Hot Environments: The Importance of Ionic Compounds For Thermostabilization", in Extremophiles Handbook, edited by K. Horikoshi, G. Antranikian, A. T. Bull, F. T. Robb, K. O. Stetter (Eds.), Part 4, pp. 497-520, Springer, Tokyo, 2011. ISBN 978-4-431-53897-4

Romão CV, Archer M, Lobo SA, Louro RO, Pereira IAC, Saraiva LM, Teixeira M, Matias P.M "Diversity of Heme Proteins in Sulfate Reducing Bacteria" in Handbook Of Porphyrin Science - With Applications to Chemistry, Physics, Materials Science, Engineering, Biology and Medicine, edited by Kadish K.M., Smith K.M. and Guilard R. 19 (89) pp 139-230, World Scientific Publishing Co. Pte. Ltd., Singapore (2012).

Scientific Papers

Noronha RG, Romao CC, Fernandes AC "A novel method for the reduction of alkenes using the system silane/oxo-rhenium complexes" Tetrahedron Lett., 51, 1048-1051 (2010). http://dx.doi.org/10.1016/j.tetlet.2009.12.061

Ascenso OS, Marques JC, Santos AR, Xavier KB, Ventura MR, Maycock CD "An efficient synthesis of the precursor of AI-2, the signalling molecule for inter-species quorum sensing", Bioorg. Med. Chem. 19 (3), 1236-41 (2011). http://dx.doi.org/10.1016/j.bmc.2010.12.036

Vyrides I, Santos H, Mingote A, Ray MJ, Stuckey DC "Are Compatible Solutes Compatible With Biological Treatment of Saline Wastewater? Batch And Continuous Studies Using Submerged Anaerobic Membrane Bioreactors (SAMBRs)". Environ. Sci. Technol. 44, 7437-7442 (2010). http://dx.doi.org/10.1021/es903981k

Collins T, Matzapetakis M, Santos H "Backbone and Side Chain 1H, 15N And 13C Assignments for a Thiol-Disulphide Oxidoreductase from The Antarctic Bacterium Pseudoalteromonas haloplanktis TAC12" Biomol NMR Assign. 4, 151-154 (2010). http://dx.doi.org/10.1007/s12104-010-9230-0

Mendes V, Maranha A, Lamosa P, da Costa MS, Empadinhas N "Biochemical characterization of the maltokinase from Mycobacterium bovis BCG" BMC Biochem. 11: 21 (2010). http://dx.doi.org/10.1186/1471-2091-11-21

Serpa J, Caiado F, Carvalho T, Torre C, Gonçalves LG, Casalou C, Lamosa P, Rodrigues M, Zhu Z, Lam EW, Dias S "Butyrate rich colonic microenvironment is a relevant selection factor for metabolically adapted tumour cells" J. Biol Chem. 285: 39211-23 (2010). http://dx.doi.org/10.1074/jbc.M110.156026

Fonseca LL, Sánchez C, Santos H, Voit EO "Complex Coordination of Multi-Scale Cellular Responses to Environmental Stress" Mol. BioSyst., 7 (3): 731-41 (2010). http://dx.doi.org/10.1039/c0mb00102c

Iranzo O, Chakraborty S, Hemmingsen L, Pecoraro VL "Controlling and Fine Tuning the Physical Properties of Two Identical Metal Coordination Sites in De Novo Designed Three Stranded Coiled Coil Peptides" J Am Chem Soc. 133 (2): 239-51 (2011). http://dx.doi.org/10.1021/ja104433n

Ribeiro JP, Palczewska M, André S, Cañada FJ, Gabius H-J, Jiménez-Barbero J, Mellström B, Naranjo JR, Scheffers DJ, Groves P "Diffusion nuclear magnetic resonance spectroscopy detects substoichiometric concentrations of small molecules in protein samples" Anal. Biochem., 396: 117-123 (2010). http://dx.doi.org/10.1016/j.ab.2009.09.001

Li F, Carvalho S, Delgado R, Drew MG, Félix V "Dimetallic complexes of macrocycles with two rigid dibenzofuran units as receptors for detection of anionic substrates" Dalton Trans. 39 9579-9587 (2010). http://dx.doi.org/10.1039/c0dt00340a

Batista AP, Fernandes AS, Louro RO, Steuber J, Pereira MM "Energy conservation by Rhodothermus marinus respiratory complex I" Biochim Biophys Acta, 1797 (4): 509-515 (2010). http://dx.doi.org/10.1016/j.bbabio.2010.01.020

Carvalho AL, Cardoso FS, Bohn A, Neves AR, Santos H "Engineering Trehalose Synthesis In Lactococcus lactis For Improved Stress Tolerance". Appl Environ Microbiol, 77 (12): 4189-4199 (2011). http://dx.doi.org/10.1128/AEM.02922-10

Carvalho S, Delgado R, Félix V "Evaluation of the binding ability of a macrobicyclic receptor for anions by potentiometry and molecular dynamics simulations in solution" Tetrahedron 66, 8714–8721 (2010). http://dx.doi.org/10.1016/j.tet.2010.09.006

Fernandes AC, Fernandes JA, Romao CC, Veiros LF, Calhorda MJ "Highly Efficient Reduction of Sulfoxides with the System Borane/Oxo-rhenium Complexes" Organometallics, 29, 5517-5525 (2010). http://dx.doi.org/10.1021/om100450a

Honzicek J, Mukhopadhyay A, Romao CC "Improved preparation of indenyl molybdenum(II) and tungsten(II) compounds" Inorganica Chimica Acta, 363, (7) 1601-1603 (2010). http://dx.doi.org/10.1016/j.ica.2010.01.022

Krishna Mohan VVK, Cardoso JMS, Peris E, Royo B "Iron(II) Complexes Bearing Chelating Cyclopentadienyl-N-Heterocyclic carbene ligands as catalysts for hydrosilylation and hydrogen transfer reactions" Organometallics 29 (12): 2777-2782 (2010). http://dx.doi.org/10.1021/om100246j

Graça J, Lamosa P "Linear and branched poly(omega-hydroxyacid) esters in plant cutins" J. Agric. Food Chem. 58, (17): 9666-9674 (2010). http://dx.doi.org/10.1021/jf1015297

Amaral AI, Teixeira AP, Martens S, Bernal V, Sousa MF, Alves PM "Metabolic alterations induced by ischemia in primary cultures of astrocytes: merging 13C NMR spectroscopy and metabolic flux analysis" J. Neurochem 113 (3): 735-748 (2010). http://dx.doi.org/10.1111/j.1471-4159.2010.06636.x

Paquete CM, Louro RO "Molecular details of multielectron transfer: the case of multiheme cytochromes from metal respiring organisms" Dalton Trans., 39, 4259-4266, (2010). http://dx.doi.org/10.1039/B917952F

Collard F, Stroobant V, Lamosa P, Kapanda CN, Lambert DM, Muccioli GG, Poupaert JH, Opperdoes F, Van Schaftingen E "Molecular identification of N-acetylaspartylglutamate synthase and β-citrylglutamate synthase" J Biol Chem., 285 (39): 29826-33 (2010). http://dx.doi.org/10.1074/jbc.M110.152629

Honzicek J, Mukhopadhyay A, Bonifacio C, Romao CC "Molybdenum complexes containing substituted cyclopenta[l]phenanthrenyl ligand". J Organomet Chem., 695, 680-686 (2010). http://dx.doi.org/10.1016/j.jorganchem.2009.11.043

Krishna Mohan VVK, Cardoso JMS, Royo B "N-heterocyclic carbene-based molybdenum and tungsten

complexes as efficient epoxidation catalysts with H2O2 and tert-butyl hydroperoxide" Catalysis Letters, 136: 222-227 (2010). http://dx.doi.org/10.1007/s10562-010-0332-1

Deive FJ, Rodríguez A, Pereiro AB, Shimizu K, Forte PA, Romão CC, Canongia Lopes JN, Esperança JM, Rebelo LP "Phase equilibria of haloalkanes dissolved in ethylsulfate- or ethylsulfonate-based ionic liquids". J Phys Chem B, 114 (21) 7329-37 (2010). http://dx.doi.org/10.1021/jp1025015

da Costa AP, Mata JA, Royo B, Peris E "Preparation of Cp-Functionalized N-Heterocyclic Carbene Complexes of Ruthenium. Resolution of chiral complexes and catalytic studies" Organometalics, 29 (7): 1832-1838 (2010). http://dx.doi.org/10.1021/om100090c

Groves P, Webba da Silva M "Rapid Stoichiometric Analysis of G-Quadruplexes in Solution" Chemistry, 16, 6451-3 (2010). http://dx.doi.org/10.1002/chem.200901248

Pokusaeva K, Neves AR, Zomer A, O'Connell-Motherway M, MacSharry J, Curley P, Fitzgerald GF, van Sinderen D "Ribose utilization by the human commensal Bifidobacterium breve UCC2003" Microb Biotechnol, 3, 311–323 (2010). http://dx.doi.org/10.1111/j.1751-7915.2009.00152.x

Cui X, Delgado R, Costa J, Drew M, Costa PJ, Félix V "Rigid Ferrocenophane and its Metal Complexes with Transition and Alkaline-earth Metal Ions" Polyhedron, 29, (6) 1697–1705 (2010). http://dx.doi.org/10.1016/j.poly.2010.02.015

Batista AP, Pereira MM "Sodium influence on energy transduction by complexes I from Escherichia coli and Paracoccus denitrificans". Biochim Biophys Acta. 1807 (3): 286-92 (2011). http://dx.doi.org/10.1016/j.bbabio.2010.12.008

Ndukum J, Fonseca LL, Santos H, Voit EO, Datta S "Statistical Inference Methods for Sparse Biological Time Series Data" BMC Systems Biology, 5: 57 (2010). http://dx.doi.org/10.1186/1752-0509-5-57

Vinga S, Neves AR, Santos H, Brandt BW, Kooijman SA "Subcellular Metabolic Organization in the Context of Dynamic Energy Budget and Biochemical Systems Theories" Philos Trans R Soc Lond B Biol Sci., 365, 3429-3442 (2010). http://dx.doi.org/10.1098/rstb.2010.0156

Lima LM, Delgado R, Marques F, Gano L, Santos I "TETA analogue containing one methylenephosphonate pendant arm: lanthanide complexes and biological evaluation of its 153Sm and 166Ho complexes" Eur J Med Chem, 45, 5621–5627 (2010). http://dx.doi.org/10.1016/j.ejmech.2010.09.013

Santos AR, Miguel AS, Tomaz L, Malhó R, Maycock C, Vaz Patto MC, Fevereiro P, Oliva A "The impact of CdSe/ZnS Quantum Dots in cells of Medicago sativa in suspension culture" J Nanobiotechnology, 8: 24 (2010). http://dx.doi.org/10.1186/1477-3155-8-24

Lourenço EC, Ventura MR "The synthesis of compatible solute analogues-solvent effects on selective glycosylation" Carbohydr Res. 346 (2): 163-8 (2011). http://dx.doi.org/10.1016/j.carres.2010.08.007

Borges N, Matsumi R, Imanaka T, Atomi H, Santos H "Thermococcus kodakaraensis Mutants Deficient in Di-myo-Inositol Phosphate use Aspartate to Cope with Heat Stress" J Bacteriol, 192, 191-197 (2010). http://dx.doi.org/10.1128/JB.01115-09

Neves AR, Pool WA, Solopova A, Kok J, Santos H, Kuipers OP "Towards Enhanced Galactose Utilization In Lactococcus lactis" Appl Environ. Microbiol., 76, 7048-7060 (2010). http://dx.doi.org/10.1128/AEM.01195-10

Fernandes C, Mendes V, Costa J, Empadinhas N, Jorge C, Lamosa P, Santos H, da Costa M "Two Alternative Pathways for the Synthesis of the Rare Compatible Solute Mannosyl-1,2-Glucosylglycerate In Petrotoga mobilis" J Bacteriol, 192, 1624-1633 (2010). http://dx.doi.org/10.1128/JB.01424-09

Alves M, Chicau P, Matias H, Passarinho J, Pinheiro C, Ricardo CP "Metabolic analysis revealed altered amino acid profiles in Lupinus albus organs due to boron deficiency" Physiol Plant. 142 (3): 224-232 (2011). http://dx.doi.org/10.1111/j.1399-3054.2011.01462.x

Araújo JM, Ferreira R, Marrucho IM, Rebelo LP "Solvation of Nucleobases in 1,3-Dialkylimidazolium Acetate Ionic Liquids: NMR Spectroscopy Insights into the Dissolution Mechanism" J. Phys. Chem. B, 115 (36): 10739-10749 (2011). http://dx.doi.org/10.1021/jp203282k

Brito JA, Borges N, Vonrhein C, Santos H, Archer M "Crystal structure of Archaeoglobus fulgidus CTP:inositol-1-phosphate cytidylyltransferase, a key enzyme for di-myo-inositol phosphate synthesis in

(hyper)thermophilic" J Bacteriol. 193 2177-2185 (2011). http://dx.doi.org/10.1128/JB.01543-10

Brito JA, Saffon N, Gómez M, Royo B "cis-Dioxomolybdenum(VI) complexes containing chiral ligands: synthesis and catalytic application in olefin epoxidation" Current Inorg. Chem, 1: 131-139 (2011). http://dx.doi.org/1877-945X/11

Campelo AB, Gaspar P, Roces C, Rodríguez A, Kok J, Kuipers OP, Neves AR, Martínez B "The Lcn972-bacteriocin plasmid pBL1 impairs cellobiose metabolism in Lactococcus lactis" Appl. Environ. Microbiol. 77 (21): 7576-7585 (2011). http://dx.doi.org/10.1128/AEM.06107-11

Carvalho SM, Kloosterman TG, Kuipers OP, Neves AR "CcpA ensures optimal metabolic fitness of Streptococcus pneumoniae" PLoS ONE 6 (10):e26707 (2011). http://dx.doi.org/10.1371/journal.pone.0026707

Chaves I, Passarinho JA, Capitão C, Chaves MM, Fevereiro P, Ricardo CP "Temperature stress effects in Quercus suber leaf metabolism" J. Plant Physiology 168: 1729-1734 (2011). http://dx.doi.org/10.1016/j.jplph.2011.05.013

da Costa AP, Lopes R, Cardoso JMS, Mata JA, Peris E, Royo B "Enantiomerically pure cyclopentadienyl- and indenyl-functionalized N-heterocyclic carbene complexes of iridium and rhodium" Organometallics, 30: 4437-4442 (2011). http://dx.doi.org/10.1021/om200523h

de Noronha RG, Romão CC, Fernandes AC "MoO2Cl2 as a novel catalyst for the synthesis of Î±-aminophosphonates" Catal. Commun 12: 337–340 (2011). http://dx.doi.org/10.1016/j.catcom.2010.10.005

Gamelas CA, Bandeira NA, Pereira CC, Calhorda MJ, Herdtweck E, Machuqueiro M, Romão CC, Veiros LF "Indenyl ring slippage in crown thioether complexes [IndMo(CO)2L]+ and C-S activation of trithiacyclononane: experimental and theoretical studies" Dalton Trans 40 (40): 10513-10525 (2011). http://dx.doi.org/10.1039/c1dt10607d

Gaspar P, Neves AR, Gasson MJ, Shearman CA, Santos H "High yields of 2,3 butanediol and mannitol in Lactococcus lactis through engineering NAD+ cofactor recycling" Appl. Environ. Microbiol. 77 (19): 6826-6835 (2011). http://dx.doi.org/10.1128/AEM.05544-11

Gonçalves S, Esteves AM, Santos H, Borges N, Matias PM "The three-dimensional structure of mannosyl-3-phosphoglycerate phosphatase from Thermus thermophilus HB27: a new member of the haloalcanoic acid dehalogenase superfamily" Biochemistry, 50 (44): 9551-9567 (2011). http://dx.doi.org/10.1021/bi201171h

Honzícek J, Romão CC, Calhorda MJ, Mukhopadhyay A, Vinklárek J, Padelková Z "Reaction of Spiro[2.4]hepta-4,6-diene with Molybdenum(II) Indenyl Compounds: Effects of Substitution in the Indenyl Ligand" Organometallics 30 (4): 717-725 (2011). http://dx.doi.org/10.1021/om100840r

Jorge CD, Ventura R, Maycock C, Outeiro TF, Santos H, Costa J "Assessment of the efficacy of solutes from extremophiles on protein aggregation in cell models of Huntington's and Parkinson's diseases" Neurochem. Res, 36 (6): 1005-1011 (2011). http://dx.doi.org/10.1007/s11064-011-0440-3

Kowacz M, Groves P, Esperança JMSS, Rebelo LPN "On the use of ionic liquids to tune crystallization" Crystal Growth & Design 11 (3): 684-691 (2011). http://dx.doi.org/10.1021/cg101061p

Lamosa P, Mingote AI, Groudieva T, Klippel B, Egorova K, Jabbour D, Santos H, Antranikian G. "Gluconeotrehalose is the principal organic solute in the psychrotolerant bacterium Carnobacterium strain 17-4" Extremophiles, 15 (4): 463-72 (2011). http://dx.doi.org/10.1007/s00792-011-0377-0

Lima MPL, Delgado R, Plutnar J, Hermann P, Kotek J "A New Tris(phosphonomethyl) Monoacetic Acid Cyclam Derivative: Synthesis, Acid-Base and Metal Complexation Studies" Eur. J. Inorg. Chem. 2011 (4): 527–538 (2011). http://dx.doi.org/10.1002/ejic.201000919

Lourenço EC, Ventura MR "Synthesis of Potassium (2R)-2-O-α-D-Mannopyranosyl-(1-2)-α-D-glucopyranosyl-2,3-dihydroxypropanoate: A natural compatible solute" Eur. J. Org. Chem, 2011 (33): 6698-6703 (2011). http://dx.doi.org/10.1002/ejoc.201100934

Marazioti A, Bucci M, Coletta C, Vellecco V, Baskaran P, Szabó C, Cirino G, Marques AR, Guerreiro B, Gonçalves AML, Seixas JD, Beuve A, Romão CC, Papapetropoulos A "Inhibition of Nitric Oxide-Stimulated Vasorelaxation by Carbon Monoxide-Releasing Molecules" Arterioscler Thromb Vasc Biol. 31 (11): 2570–2576 (2011). http://dx.doi.org/10.1161/ATVBAHA.111.229039

Marques JC, Lamosa P, Russell C, Ventura R, Maycock C, Semmelhack MF, Miller ST, Xavier KB “Processing the interspecies quorum-sensing signal autoinducer-2 (AI-2): characterization of phospho-(S)-4,5-dihydroxy-2,3-pentanedione isomerization by LsrG protein” J Biol Chem, 286: 18331-43 (2011). http://dx.doi.org/10.1074/jbc.M111.230227

Mateus P, Delgado R, Brandão P, Félix V “Recognition of oxalate by a copper(II) polyaza macrobicyclic complex” Chemistry 17 (25): 7020-7031 (2011). http://dx.doi.org/10.1002/chem.201100428

Mateus P, Delgado R, Lloret F, Cano J, Brandão P, Félix V ”A trinuclear copper(II) cryptate and its μ3-CO3 cascade complex: thermodynamics, structural and magnetic properties” Chemistry, 17 (40) :11193-11203 (2011). http://dx.doi.org/10.1002/chem.201101372

Mateus P, Li F, Esteves CV, Delgado R, Brandão P, Félix V “Properties of metal complexes of a new dioxadiaza macrocycle containing a dibenzofuran unit and acetate pendant arms” Eur. J. Inorg. Chem. 2011 (30): 4700–4708 (2011). http://dx.doi.org/10.1002/ejic.201100612

Müller S, Hoffmann T, Santos H, Saum SH, Bremer E, Müller V “Bacterial abl-like genes: production of the archaeal osmolyte N(ε)-acetyl-β-lysine by homologous overexpression of the yodP-kamA genes in Bacillus subtilis” Appl. Microbiol. Biotechnol. 91 (3): 689-697 (2011). http://dx.doi.org/10.1007/s00253-011-3301-8

Reinstein O, Neves MA, Saad M, Boodram SN, Lombardo S, Beckham SA, Brouwer J, Audette GF, Groves P, Wilce MC, Johnson PE “Engineering a Structure Switching Mechanism into a Steroid-Binding Aptamer and Hydrodynamic Analysis of the Ligand Binding Mechanism”, Biochemistry 50: 9368-9376 (2011). http://dx.doi.org/10.1021/bi201361v

Reis PM, Gamelas CA, Brito JA, Saffon N, Gómez M, Royo B “Chiral Cationic [Cp´Mo(CO)2(NCMe)]+ Species: Catalyst Precursors for Olefin Epoxidation with H2O2 and tert-Butyl Hydroperoxide” Eur. J. Inorg. Chem, 2011 (5): 666-673 (2011). http://dx.doi.org/10.1002/ejic.201001065

Rodrigues CAB, de Matos MN, Guerreiro BMH, Goncalves AML, Romão CC, Afonso CAM “Water as efficient medium for mild decarbonylation of tertiary aldehydes” Tetrahedron Letters 52 (22): 2803-2807 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.03.012

Sand M, de Berardinis V, Mingote A, Santos H, Göttig S, Müller V, Averhoff B “Salt adaptation in Acinetobacter baylyi: identification and characterization of a secondary glycine betaine transporter” Arch Microbiol. 193 (10): 723-730 (2011). http://dx.doi.org/10.1007/s00203-011-0713-x

Batista AP, Marreiros BC, Louro RO, Pereira MM. “Study of ion translocation by respiratory complex I. A new insight using 23Na NMR spectroscopy” Biochim Biophys Acta 1817 (10): 1810-1816 (2012). http://dx.doi.org/10.1016/j.bbabio.2012.03.009

Bernier N, Esteves CV, Delgado R. "Heteroditopic receptor based on crown ether and cyclen units for the recognition of zwitterionic amino acids", Tetrahedron 68 (24): 4860–4868 (2012). http://dx.doi.org/10.1016/j.tet.2012.03.110

Cardoso JMS, Royo B “Unprecedented synthesis of iron-NHC complexes by C-H activation of imidazolium salts. Mild catalysts for reduction of sulfoxides” Chem. Commun. 48 (41): 4944-4946 (2012). http://dx.doi.org/10.1039/c2cc31564e

Ferreira R, Garcia H, Sousa AF, Petkovic M, Lamosa P, Freire C, Silvestre AJD, Rebelo LPN, Silva-Pereira C “Suberin isolation process from cork using ionic liquids: characterisation of ensuing products” New J. Chem., 36: 2014-2024 (2012). http://dx.doi.org/10.1039/C2NJ40433H

Ferreira R, Garcia H, Sousa AF, Freire CSR, Silvestre AJD, Rebelo LPN, Silva-Pereira C “Isolation of suberin from birch outer bark and cork using ionic liquids: A new source of macromonomers” Ind Crops Prod 44: 520-527 (2013). http://dx.doi.org/10.1016/j.indcrop.2012.10.002

Fonseca BM, Tien M, Rivera M, Shi L, Louro RO “Efficient and selective isotopic labeling of hemes to facilitate the study of multiheme proteins” Biotechniques 0 (0): 1-7 (2012). http://dx.doi.org/10.2144/000113859

Gamelas CA, Gomes AC, Bruno SM, Paz FAA, Valente AA, Pillinger M, Romão CC, Gonçalves IS “Molybdenum(VI) catalysts obtained from eta(3)-allyl dicarbonyl precursors: Synthesis, characterization and catalytic performance in cyclooctene epoxidation” Dalton Trans. 41 (12): 3474–3484 (2012). http://dx.doi.org/10.1039/c2dt11751g

Gamelas CA, Neves P, Gomes AC, Valente AA, Romão CC, Gonçalves IS, Pillinger M “Molybdenum(II) Diiodo-Tricarbonyl Complexes Containing Nitrogen Donor Ligands as Catalyst Precursors for the Epoxidation of Methyl

Oleate" Catal Lett 142 (10): 1218–1224 (2012). http://dx.doi.org/10.1007/s10562-012-0890-5

Lima LMP, Delgado R, Hermann P, Ševčík R, Lubal P, Carvalho HF, Martins AF, Tóth É, Geraldes CFGC "Tris(phosphonomethyl) cyclen derivatives: 2) Thermodynamic stability, kinetics, solution structure, and relaxivity of Ln3+ complexes", Eur. J. Inorg. Chem., 2012 (15): 2548–2559 (2012). http://dx.doi.org/10.1002/ejic.201101335

Lima LMP, Esteves CV, Delgado R, Hermann P, Kotek J, Ševčíková R, Lubal P "Tris(phosphonomethyl) cyclen derivatives: 1) Synthesis, acid-base properties, and complexation studies with Cu2+ and Zn2+ ions" Eur. J. Inorg. Chem., 2012 (15): 2533–2547 (2012). http://dx.doi.org/10.1002/ejic.201101334

Louro RO, Paquete CM "The quest to achieve the detailed structural and functional characterization of CymA" Biochem Soc Trans 40 (6), 1291-1294 (2012). http://dx.doi.org/10.1042/BST20120114

Maiti BK, Aviles T, Matzapetakis M, Moura I, Pauleta SR, Moura JJG "Synthesis of [MoS4]2--M (M = Cu and Cd) Clusters: Potential NMR Spectroscopic Structural Probes for the Orange Protein" European Journal of Inorganic Chemistry 2012 (26): 4159-4166 (2012). http://dx.doi.org/10.1002/ejic.201200551

Marques AR, Kromer L, Gallo DJ, Penacho N, Rodrigues SS, Seixas JD, Bernardes GJL, Reis PM, Otterbein SL, Ruggieri RA, Gonçalves ASG, Gonçalves AML, Matos MND, Bento I, Otterbein LE, Blattler WA, Romão CC "Generation of Carbon Monoxide Releasing Molecules (CO-RMs) as Drug Candidates for the Treatment of Acute Liver Injury: Targeting of CO-RMs to the Liver" Organometallics 31 (16), 5810-5822 (2012). http://dx.doi.org/10.1021/om300360c

Mateus P, Delgado R, Brandão P, Félix V "A polyoxapolyaza macrobicyclic receptor for the recognition of zwitterions", Org. Biomol. Chem. 10, 5529–5532 (2012). http://dx.doi.org/10.1039/C2OB25725D

Mateus P, Delgado R, Brandão P, Félix V "Dicarboxylate recognition by two macrobicyclic receptors: selectivity for fumarate over maleate", J. Org. Chem. 77 (10): 4611–4621 (2012). http://dx.doi.org/10.1021/jo300320w

Mateus P, Delgado R, Groves P, Campos SRR, Baptista AM, Brandão P, Félix V "Water encapsulation in a polyoxapolyaza macrobicyclic compound", J. Org. Chem. 77 (16), 6816–6824 (2012). http://dx.doi.org/10.1021/jo300799s

Maycock CD, Ventura MR "New organocatalysts derived from tartaric and glyceric acids for direct aldol reactions" Tetrahedron: Asymmetry 23 (17): 1262-1271 (2012). http://dx.doi.org/10.1016/j.tetasy.2012.08.008

Nobre A, Empadinhas N, Nobre MF, Lourenço EC, Maycock C, Ventura MR, Mingote A, da Costa MS "The plant Selaginella moellendorffii possesses enzymes for synthesis and hydrolysis of the compatible solutes mannosylglycerate and glucosyslglycerate" Planta [Epub ahead of print] (2012). http://dx.doi.org/10.1007/s00425-012-1808-6

Nóbrega CS, Matzapetakis M, Pauleta SR "(1)H, (13)C and (15)N resonance assignment of the soluble form of the Lipid-modified Azurin from Neisseria gonorrhoeae" Biomol NMR Assign. [Epub ahead of print] (2012). http://dx.doi.org/10.1007/s12104-012-9434-6

Pais TM, Lamosa P, Matzapetakis M, Turner DL, Santos H "Mannosylglycerate stabilizes staphylococcal nuclease with restriction of slow β-sheet motions" Protein Science 21 (8): 1126-1137 (2012). http://dx.doi.org/10.1002/pro.2100

Pena AC, Penacho N, Mancio-Silva L, Neres R, Seixas JD, Fernandes AC, Romão CC, Mota MM, Bernardes GJL, Pamplona A "A Novel Carbon Monoxide-Releasing Molecule Fully Protects Mice from Severe Malária" Antimicrob Agents Chemother. 56 (3): 1281–1290 (2012). http://dx.doi.org/10.1128/AAC.05571-11

Pereira CS, Santos AJM, Bejerano-Sagie M, Correia PB, MarquesJC, Xavier KB "Phosphoenolpyruvate Phosphotransferase System regulates detection and processing of the quorum sensing signal Autoinducer-2" Mol. Microbiol. 84 (1): 93-104 (2012). http://dx.doi.org/10.1111/j.1365-2958.2012.08010.x

Petkovic M, Hartmann DO, Adamova G, Seddon KR, Rebelo LPN, Silva-Pereira C "Unravelling the mechanism of toxicity of alkyltributylphosphonium chlorides in Aspergillus nidulans conidia" New J Chem, 36, 56–63 (2012). http://dx.doi.org/10.1039/C1NJ20470J

Pires S, Habjanič J, Sezer M, Soares CM, Hemmingsen L, Iranzo O "Design of a Peptidic Turn with High Affinity for HgII" Inorg. Chem. 51 (21), 11339-11348 (2012). http://dx.doi.org/10.1021/ic3008014

Postigo L, Royo B “N- Heterocyclic carbene complexes of nickel as efficient catalysts for hydrosilylation of carbonyl derivatives” Adv. Synth. Catal. 354 (14-15): 2613-2618 (2012). http://dx.doi.org/10.1002/adsc.201200389

Pottabathula S, Royo B “First iron-catalyzed guanylation of amines: a simple and highly efficient protocol to guanidines” Tetrahedron Lett. 53 (38), 5156-5158 (2012). http://dx.doi.org/10.1016/j.tetlet.2012.07.065

Rodrigues F, Sousa MJ, Ludovico P, Santos H, Côrte-Real M, Leão C “The fate of acetic acid during glucose co-metabolism by the spoilage yeast Zygosaccharomyces bailli”. PLOS One, 7 (12): e52402 (2012). http://dx.doi.org/10.1371/journal.pone.0052402

Rui F, Marques JC, Miller ST, Maycock CD, Xavier KB, Ventura MR “Stereochemical diversity of AI-2 analogs modulates quorum sensing in Vibrio Harveyi and Escheria coli” Bioorg. Med. Chem., 20 (1): 249-256 (2012). http://dx.doi.org/10.1016/j.bmc.2011.11.007

Santos MFA, Seixas JD, Coelho AC, Mukhopadhyay A, Reis PM, Romão MJ, Romão CC, Santos-Silva T “New insights into the chemistry of fac-[Ru(CO)3]2+ fragments in biologically relevant conditions: The CO releasing activity of [Ru(CO)3Cl2(1,3-thiazole)], and the X-ray crystal structure of its adduct with lysozyme” J Inorg Biochem 117, 285–291 (2012). http://dx.doi.org/10.1016/j.jinorgbio.2012.06.018

Saraiva IH, Newman DK, Louro RO “Functional characterization of the FoxE iron oxidoreductase from the photoferrotroph Rhodobacter ferrooxidans SW2” J Biol Chem, 287 (30): 25541-25548 (2012). http://dx.doi.org/10.1074/jbc.M112.360636

Solopova A, Bachmann H, Teusink B, Kok J, Neves AR, Kuipers OP “A specific mutation in the promoter region of the silent cel cluster accounts for the appearance of lactose-utilizing Lactococcus lactis MG1363” Appl Environ Microbiol. 78 (16): 5612-5621 (2012). http://dx.doi.org/10.1128/AEM.00455-12

Turner DL, Catarino T “Homotropic and heterotropic interactions in cytochromes c(3) from sulphate reducing bacteria” FEBS Letters 586 (5): 494-503 (2012). http://dx.doi.org/10.1016/j.febslet.2011.07.007

Vicente A, Caio J, Sardinha J, Moiteiro C, Delgado R, Félix V "Evaluation of the binding ability of tetraaza[2]arene[2]triazine receptors anchoring L-alanine units for aromatic carboxylate anions" Tetrahedron 68 (2): 670–680 (2012). http://dx.doi.org/10.1016/j.tet.2011.10.090

Emília Leitão, Christopher Maycock, Rita Ventura (2012) “Method for the preparation of biologically active compounds” Hovione, Patent PCT/2012/000469 (PT105723).

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Book Chapters

Gil AM “Metabonomics in Food Science” in Encyclopedia of Spectroscopy and Spectrometry, 2nd Edition, Chapter 5, Elsevier, Oxford, pp. 1513-1520, 2010.

Paz FAA, Rocha J “N-(phosphonomethyl)iminodiacetic acid in the construction of Coordination polymers”, in Metal Phosphonate Chemistry: From Synthesis to Applications (Chapter 17), Royal Society of Chemistry, Edited by Abraham Clearfield and Konstantinos Demadis, 2011.

Mafra L, Vidal-Moya JA, Blasco T “Structural characterization of zeolites by advanced solid-state NMR spectroscopic methods” in Annual Reports on NMR Spectroscopy, Series Editor: Graham Webb, Royal Society of Chemistry, Burlington House, London, UK, Vol. 70 (2012) 259-351. ISBN 13: 978-0-12-381353-4

Scientific Papers

Ait-Baziz N, Rachedi Y, Silva AMS “Reactivity of some structural analogs of dehydroacetic acid with o-phenylenediamine” Arkivoc X, 86-97 (2010). ISSN 1551-7012

Alkorta I, Elguero J, Silva AMS, Tomé AC “A theoretical study of the conformation of meso-tetraphenylporphyrin (TPPH2), its anions, cations and metal complexes (Mg2+, Ca2+ and Zn2+)”. Journal of Porphyrins and Phthalocyanines, 14, (7), 630-638 (2010). http://dx.doi.org/10.1142/S1088424610002409

Almeida AIS, Silva AMS, Cavaleiro JAS “Reactivity of 3-Iodo-4-quinolones in Heck Reactions: Synthesis of Novel (E)-3-Styryl-4-quinolones” Synlett 2010, (3), 462-466 (2010). http://dx.doi.org/10.1055/s-0029-1219175

Amghouz Z, Roces L, García-Granda S, Garcia JR, Souhail B, Mafra L, Shi FN, Rocha J "Metal Organic Frameworks Assembled from Y(III), Na(I), and Chiral Flexible-Achiral Rigid Dicarboxylates" Inorganic Chemistry 49, (17), 7917-7926 (2010). http://dx.doi.org/10.1021/ic100867w

Barata JFB, Neves M, Tomé AC, Faustino MAF, Silva AMS, Cavaleiro JAS "How light affects 5,10,15-tris(pentafluorophenyl)corrole" Tetrahedron Letters 51, (12), 1537-1540 (2010). http://dx.doi.org/10.1016/j.tetlet.2010.01.033

Borrego T, Andrade M, Pinto ML, Silva AR, Carvalho AP, Rocha J, Freire C, Pires J. "Physicochemical characterization of silylated functionalized materials" J Colloid Interface Sci. 344 (2), 603-610 (2010). http://dx.doi.org/10.1016/j.jcis.2010.01.026

Carvalho ARF, Oliveira J, de Freitas V, Silva A, Mateus N, Melo A "A computational study of vinylpyranoanthocyanin-phenolic pigments (portisins)" Journal of Molecular Structure: THEOCHEM 946, (1-3), 113-118 (2010). http://dx.doi.org/10.1016/j.theochem.2009.07.034

Castro A, Alonso JC, Valente AA, Neves P, Brandão P, Félix V, Ferreira P "Nanostructured dioxomolybdenum(VI) catalyst for the liquid-phase epoxidation of olefins" European Journal of Inorganic Chemistry 2010, 1405–1412 (2010). http://dx.doi.org/10.1002/ejic.200901093

Castro A, Alonso JC, Neves P, Valente AA, Ferreira P "Dioxomolybdenum(VI) epoxidation catalyst supported on a mesoporous silica containing phosphane oxide groups" European Journal of Inorganic Chemistry 2010, 602–607 (2010). http://dx.doi.org/10.1002/ejic.200900918

Coelho AC, Balula SS, Antunes MM, Gerganova TI, Bion N, Ferreira P, Pillinger M, Valente AA, Rocha J, Gonçalves IS "Complexation of crystal-like mesoporous phenylene-silica with Cr(CO)3 and catalytic performance in the oxidation of cyclooctene" Journal of Molecular Catalysis A - Chemical 332 (1-2) 13-18 (2010). http://dx.doi.org/10.1016/j.molcata.2010.08.010

Coelho AC, Balula SS, Bruno SM, Alonso JC, Bion N, Ferreira P, Pillinger M, Valente AA, Rocha J, Goncalves IS "Grafting of Molecularly Ordered Mesoporous Phenylene-Silica with Molybdenum Carbonyl Complexes: Efficient Heterogeneous Catalysts for the Epoxidation of Olefins" Advanced Synthesis & Catalysis 352, (10), 1759-1769 (2010). http://dx.doi.org/10.1002/adsc.201000042

Costa T, Seixas de Melo J, Castro CS, Gago S, Pillinger M, Gonçalves IS. "Picosecond Dynamics of Dimer Formation in a Pyrene Labeled Polymer" J Phys Chem B. 114, 12439-12447 (2010). http://dx.doi.org/10.1021/jp1020214

Cunha AC, Gomes A, Ferreira VF, de Souza M, Neves M, Tomé AC, Silva AMS, Cavaleiro JAS. "Synthesis of β-Arylporphyrins and Oligophenylenediporphyrins by the Suzuki-Miyaura Reaction" Synthesis 2010, (3), 510-514 (2010). http://dx.doi.org/10.1055/s-0029-1217114

Duarte IF, Lamego I, Marques J, Marques MPM, Blaise BJ, Gil AM. "Nuclear Magnetic Resonance (NMR) Study of the Effect of Cisplatin on the Metabolic Profile of MG-63 Osteosarcoma Cells" J Proteome Res. 9, (11), 5877-5886 (2010). http://dx.doi.org/10.1021/pr100635n

Duarte IF, Rocha CM, Barros AS, Gil AM, Goodfellow BJ, Carreira IM, Bernardo J, Gomes A, Sousa V, Carvalho L. "Can nuclear magnetic resonance (NMR) spectroscopy reveal different metabolic signatures for lung tumours?" Virchows Arch.457, (6), 715-25 (2010). http://dx.doi.org/10.1007/s00428-010-0993-6

Ferreira JA, Azevedo NF, Vieira MJ, Figueiredo C, Goodfellow BJ, Monteiro MA, Coimbra MA. "Identification of cell-surface mannans in a virulent Helicobacter pylori strain" Carbohydr Res. 345, (6), 830-838 (2010). http://dx.doi.org/10.1016/j.carres.2010.01.022

Freire MG, Neves C, Silva AMS, Santos L, Marrucho IM, Rebelo LPN, Shah JK, Maginn EJ, Coutinho JAP. "1H NMR and Molecular Dynamics Evidence for an Unexpected Interaction on the Origin of Salting-In/Salting-Out Phenomena" J Phys Chem B. 114, (5), 2004-14 (2010). http://dx.doi.org/10.1021/jp9095634

García-Granda S, Khainakov SA, Espina A, Garcia JR, Castro GR, Rocha J, Mafra L. "Revisiting the Thermal Decomposition of Layered γ-Titanium Phosphate and Structural Elucidation of Its Intermediate Phases" Inorg Chem 49, (6), 2630-2638 (2010). http://dx.doi.org/10.1021/ic901254j

Graca G, Duarte IF, Barros AS, Goodfellow BJ, Diaz SO, Pinto J, Carreira IM, Galhano E, Pita C, Gil AM. "Impact of Prenatal Disorders on the Metabolic Profile of Second Trimester Amniotic Fluid: A Nuclear Magnetic Resonance Metabonomic Study" J Proteome Res. 9, (11), 6016-24 (2010). http://dx.doi.org/10.1021/pr100815q

Lima MRM, Felgueiras ML, Graca G, Rodrigues JEA, Barros A, Gil AM, Dias ACP. "NMR metabolomics of esca

disease-affected Vitis vinifera cv. Alvarinho leaves" J Exp Bot. 61, (14), 4033-4042 (2010). http://dx.doi.org/10.1093/jxb/erq214

Lima S, Antunes MM, Fernandes A, Pillinger M, Ribeiro MF, Valente AA. "Catalytic Cyclodehydration of Xylose to Furfural in the Presence of Zeolite H-Beta and a Micro/Mesoporous Beta/TUD-1 Composite Material" Applied Catalysis A: General 388, 141-148 (2010). http://dx.doi.org/10.1016/j.apcata.2010.08.040

Lima S, Antunes MM, Fernandes A, Pillinger M, Ribeiro MF, Valente AA. "Acid-Catalysed Conversion of Saccharides into Furanic Aldehydes in the Presence of Three-Dimensional Mesoporous Al-TUD-1" Molecules 15, 3863-3877 (2010). http://dx.doi.org/10.3390/molecules15063863

Micaelo, NM; Macedo, AL; Goodfellow, BJ, Felix V "Tetrapyrrole binding affinity of the murine and human p22HBP heme-binding proteins" J. Mol. Graph Model. 29, 3: 396-405 (2010). http://dx.doi.org/10.1016/j.jmgm.2010.07.008

Monteiro B, Cunha-Silva L, Gago S, Klinowski J, Paz FAA, Rocha J, Goncalves IS, Pillinger M. "Crystal and supramolecular structures of dioxomolybdenum(VI) and dioxotungsten(VI) complexes of dihydroxybenzoic acids" Polyhedron 29, (2), 719-730 (2010). http://dx.doi.org/10.1016/j.poly.2009.10.015

Moura NMM, Giuntini F, Faustino MAF, Neves M, Tomé AC, Silva AMS, Rakib EM, Hannioui A, Abouricha S, Roder B, Cavaleiro JAS. "1,3-Dipolar cycloaddition of nitrile imines to meso-tetraarylporphyrins" Arkivoc 2010, (V), 24-33 (2010). ISSN: 1551-7012

Oliva CG, Silva AMS, Paz FAA, Cavaleiro JAS. "Highly Enantioselective and Regioselective Conjugate Addition of Nitromethane to 1,5-Diarylpenta-2,4-dien-1-ones Using Bifunctional Cinchona Organocatalysts" Synlett 2010, (7), 1123-1127 (2010). http://dx.doi.org/10.1055/s-0029-1219576

Oliva CG, Silva AMS, Resende D, Paz FAA, Cavaleiro JAS. "Highly Enantioselective 1,4-Michael Additions of Nucleophiles to Unsaturated Aryl Ketones with Organocatalysis by Bifunctional Cinchona Alkaloids" Eur. J Org. Chem. 2010, (18), 3449-3458 (2010). http://dx.doi.org/10.1002/ejoc.201000273

Paixão V, Carvalho AP, Rocha J, Fernandes A, Martins A. "Modification of MOR by desilication treatments: Structural, textural and acidic characterization" Microporous and Mesoporous Materials 131, (1-3), 350-357 (2010). http://dx.doi.org/10.1016/j.micromeso.2010.01.013

Patoilo DT, Silva AMS, Cavaleiro JAS. "Regioselective 3-Nitration of Flavones: A New Synthesis of 3-Nitro- and 3-Aminoflavones" Synlett 2010, (9), 1381-85 (2010). http://dx.doi.org/10.1055/s-0029-1219838

Patonay T, Vasas A, Kiss-Szikszai A, Silva AMS, Cavaleiro JAS. "Efficient Synthesis of Chromones with Alkenyl Functionalities by the Heck Reaction" Australian Journal of Chemistry 63, (11), 1582-1593 (2010). http://dx.doi.org/10.1071/CH10295

Pinho SLC, Pereira GA, Voisin P, Kassem J, Bouchaud V, Etienne L, Peters JA, Carlos LD, Mornet S, Geraldes C, Rocha J, Delville MH. "Fine Tuning of the Relaxometry of -γ-Fe2O3@SiO2 Nanoparticles by Tweaking the Silica Coating Thickness" ACS Nano 4, (9), 5339-49 (2010). http://dx.doi.org/10.1021/nn101129r

Resende D, Oliva CG, Silva AMS, Paz FAA, Cavaleiro JAS. "Domino Multicomponent Michael-Michael-Aldol Reactions under Phase-Transfer Catalysis: Diastereoselective Synthesis of Pentasubstituted Cyclohexanes" Synlett 2010, (1), 115-118 (2010). http://dx.doi.org/10.1055/s-0029-1218523

Rocha CM, Barros AS, Gil AM, Goodfellow BJ, Humpfer E, Spraul M, Carreira IM, Melo JB, Bernardo J, Gomes A, Sousa V, Carvalho L, Duarte IF. "Metabolic Profiling of Human Lung Cancer Tissue by 1H High Resolution Magic Angle Spinning (HRMAS) NMR Spectroscopy" J Proteome Res 9, (1), 319-332 (2010). http://dx.doi.org/10.1021/pr9006574

Rocha J, Shi FN, Paz FAA, Mafra L, Sardo M, Cunha-Silva L, Chisholm J, Ribeiro-Claro P, Trindade T. "3D-2D-0D Stepwise Deconstruction of a Water Framework Templated by a Nanoporous Organic-Inorganic Hybrid Host" Chemistry 16, (26), 7741-7749 (2010). http://dx.doi.org/10.1002/chem.201000431

Rocha-Pereira J, Cunha R, Pinto D, Silva AMS, Nascimento MS. "(E)-2-Styrylchromones as potential anti-norovirus agents" Bioorg Med Chem. 18, (12), 4195-4201 (2010). http://dx.doi.org/10.1016/j.bmc.2010.05.006

Rodrigues JE, Erny GL, Barros AS, Esteves VI, Brandão T, Ferreira AA, Cabrita EJ, Gil AM "Quantification of organic acids in beer by nuclear magnetic resonance (NMR)-based

methods" Anal. Chim Acta, 674 (2): 166-175 (2010). http://dx.doi.org/10.1016/j.aca.2010.06.029

Santos CMM, Freitas M, Ribeiro D, Gomes A, Silva AMS, Cavaleiro JAS, Fernandes E. "2,3-Diarylxanthones as strong scavengers of reactive oxygen and nitrogen species: A structure-activity relationship study" Bioorg Med Chem 18, (18), 6776-6784 (2010). http://dx.doi.org/10.1016/j.bmc.2010.07.044

Seca AML, Silva AMS. "A new 4',7-epoxy-8,3'-oxyneolignan from the acetone extract of Juniperus brevifolia leaves" Phytochemistry Letters 3, (3) 126-128 (2010). http://dx.doi.org/10.1016/j.phytol.2010.04.002

Seixas R, Silva AMS, Cavaleiro JAS. "New Synthesis of (Z)- and (E)-3-Styryl-4-quinolones" Synlett 2010, (15), 2257-2262 (2010). http://dx.doi.org/10.1055/s-0030-1258042

Silva VLM, Silva AMS, Cavaleiro JAS. "New Synthesis of 2,3-Diarylacridin-9(10H)-ones and (E)-2-Phenyl-4-styrylfuro[3,2-c]quinolines" Synlett 2010, (17), 2565-2570 (2010). http://dx.doi.org/10.1055/s-0030-1258579

Silva VLM, Silva AMS, Pinto D, Rodriguez P, Gomez M, Jagerovic N, Callado LF, Cavaleiro JAS, Elguero J, Fernandez-Ruiz J. "Synthesis and pharmacological evaluation of new (E)- and (Z)-3-aryl-4-styryl-1H-pyrazoles as potential cannabinoid ligands" Arkivoc 2010 (X), 226-247 (2010). ISSN: 1551-7012

Webber AL, Elena B, Griffin JM, Yates JR, Pham TN, Mauri F, Pickard CJ, Gil AM, Stein R, Lesage A, Emsley L, Brown SP. "Complete 1H resonance assignment of β-maltose from 1H-1H DQ-SQ CRAMPS and 1H (DQ-DUMBO)-13C SQ refocused INEPT 2D solid-state NMR spectra and first principles GIPAW calculations" Phys Chem Chem Phys. 12, (26), 6970-6983 (2010). http://dx.doi.org/10.1039/c001290d

Almeida AIS, Silva AMS, Cavaleiro JAS. "4-Chloro-3-iodoquinoline as a Synthon in the Development of New Syntheses of 1,2-Disubstituted 1H-Pyrrolo[3,2-c]quinolines". Synlett 2011, (20) 2955-2958 (2011). http://dx.doi.org/10.1055/s-0031-1289909

Arrojado C, Pereira C, Tomé JPC, Faustino MAF, Neves M, Tomé AC, Cavaleiro JAS, Cunha A, Calado R, Gomes NCM, Almeida A. "Applicability of photodynamic antimicrobial chemotherapy as an alternative to inactivate fish pathogenic bacteria in aquaculture systems". Photochem Photobiol Sci. 10, (10), 1691-1700 (2011). http://dx.doi.org/10.1039/c1pp05129f

Ay AN, Zumreoglu-Karan B, Temel A, Mafra L. "Layered double hydroxides with interlayer borate anions: A critical evaluation of synthesis methodology and pH-independent orientations in nano-galleries". Applied Clay Science 51, (3), 308-316 (2011). http://dx.doi.org/10.1016/j.clay.2010.12.015

Carrola J, Rocha CM, Barros AS, Gil AM, Goodfellow BJ, Carreira IM, Bernardo J, Gomes A, Sousa V, Carvalho L, Duarte IF "Metabolic Signatures of Lung Cancer in Biofluids: NMR-Based Metabonomics of Urine" J Proteome Res 10, (1), 221-230 (2011). http://dx.doi.org/10.1021/pr100899x

Carvalho CMB, Neves M, Tomé AC, Paz FAA, Silva AMS, Cavaleiro JAS. "1,3-Dioxopyrrolo[3,4-b]porphyrins: Synthesis and Chemistry" Org Lett. 13, (1), 130-133 (2011). http://dx.doi.org/10.1021/ol102691s

Costa JIT, Tomé AC, Neves MGPMS, Cavaleiro JAS. "5,10,15,20-Tetrakis(pentafluorophenyl)porphyrin: a versatile platform to novel porphyrinic materials" Journal of Porphyrins and Phthalocyanines 15, 1116-1133 (2011). http://dx.doi.org/10.1142/S1088424611004294

De Paula R, Simões MMQ, Neves M, Cavaleiro JAS "Oxidation of styrene and of some derivatives with H2O2 catalyzed by novel imidazolium-containing manganese porphyrins: A mechanistic and thermodynamic interpretation". Journal of Molecular Catalysis A: Chemical 345, (1-2), 1-11 (2011). http://dx.doi.org/10.1016/j.molcata.2011.05.013

Diaz SO, Pinto J, Graca G, Duarte IF, Barros AS, Galhano E, Pita C, Almeida MD, Goodfellow BJ, Carreira IM, Gil AM. "Metabolic Biomarkers of Prenatal Disorders: An Exploratory NMR Metabonomics Study of Second Trimester Maternal Urine and Blood Plasma". Journal of Proteome Research 10, (8), 3732-3742 (2011). http://dx.doi.org/10.1021/pr200352m

Duarte IF. "Following dynamic biological processes through NMR-based metabonomics: A new tool in nanomedicine?" J Control Release 153, (1), 34-39 (2011). http://dx.doi.org/10.1016/j.jconrel.2011.03.008

El Maatougui A, Crespo A, Silva AMS, Coelho A. "Supported TBD-Assisted Solution Phase Diversification of Formyl-Aza-Heterocycles Through Alkylation-Knoevenagel One Pot Sequences" Combinatorial Chemistry & High

Throughput Screening 14, (7), 570-582 (2011). ISSN: 1875-5402

Esteves CIC, Santos CMM, Brito CM, Silva AMS, Cavaleiro JAS. "Synthesis of Novel 1-Aryl-9H-xanthen-9-ones" Synlett 2011, (10), 1403-1406 (2011). http://dx.doi.org/10.1055/s-0030-1260567

Estrada AC, Santos I, Simões MMQ, Neves M, Cavaleiro JAS, Cavaleiro AMV. "Silica supported transition metal substituted polyoxotungstates: Novel heterogeneous catalysts in oxidative transformations with hydrogen peroxide". Applied Catalysis A-General 392, (1-2), 28-35 (2011). http://dx.doi.org/10.1016/j.apcata.2010.10.026

Estrada AC, Simões MMQ, Santos I, Neves M, Cavaleiro JAS, Cavaleiro AMV. "Oxidation of Polycyclic Aromatic Hydrocarbons with Hydrogen Peroxide in the Presence of Transition Metal Mono-Substituted Keggin-Type Polyoxometalates". ChemCatChem 3, (4), 771-779 (2011). http://dx.doi.org/10.1002/cctc.201000264

Fernandes JA, Paz FAA, Braga SS, Ribeiro-Claro PJA, Rocha J. "Inclusion of potassium 4,4'-biphenyldicarboxylate into β-cyclodextrin: the design and synthesis of an organic secondary building unit" New Journal of Chemistry 35, (6), 1280-1290 (2011). http://dx.doi.org/10.1039/C0NJ00796J

Fernandes M, Nobre SS, Xu QH, Carcel C, Cachia JN, Cattoën X, Sousa JM, Ferreira RAS, Carlos LD, Santilli CV, Man MWC, Bermudez VD. "Self-Structuring of Lamellar Bridged Silsesquioxanes with Long Side Spacers" J Phys Chem B. 115, (37), 10877-91 (2011). http://dx.doi.org/10.1021/jp2022902

Ferreira A, Lin Z, Soares MR, Rocha J "Novel microporous zirconium silicate (K2ZrSi3O9·2H2O) from high temperature phase transformation" Journal of Solid State Chemistry 183, (12), 3067-3072 (2011). http://dx.doi.org/10.1016/j.jssc.2010.10.013

Figueira F, Cavaleiro JAS, Tomé JPC, "Silica nanoparticles functionalized with porphyrins and analogs for biomedical studies" Journal of Porphyrins and Phthalocyanines 15, (7-8), 517-533 (2011). http://dx.doi.org/10.1142/S1088424611003653

Gomes A, Cunha AC, Domingues MDM, Neves M, Tomé AC, Silva AMS, Santos FD, Souza M, Ferreira VF, Cavaleiro JAS. "Synthesis and characterization of new porphyrin/4-quinolone conjugates" Tetrahedron 67, (38), 7336-7342 (2011). http://dx.doi.org/10.1016/j.tet.2011.07.025

Gomes A, Neves M, Cavaleiro JAS. "Diazo compounds in the functionalization of porphyrin macrocycles" Journal of Porphyrins and Phthalocyanines 15, (9-10), 835-847 (2011). http://dx.doi.org/10.1142/S1088424611003884

Gomes A, Paz FAA, Neves M, Tomé AC, Silva AMS, de Souza M, Ferreira VF, Cavaleiro JAS. "Catalytic carbene insertion into an aminoporphyrin and formation of a new chiral supramolecular porphyrin system" Tetrahedron Letters 52, (37), 4741-4744 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.06.120

Hikem-Oukacha D, Hamdi M, Silva AMS, Yahia R. "New Synthesis and Reactivity of 3-Bromoacetyl-4-hydroxy-6-methyl-2H-pyran-2-one with Binucleophilic Amines" Journal of Heterocyclic Chemistry 48, (1), 63-68 (2011). http://dx.doi.org/10.1002/jhet.507

Hikem-Oukacha D, Rachedi Y, Hamdi M, Silva AMS. "Synthesis and Reactivity of 6-MethyL-4H-furo[3,2c]pyran-3,4-dione" Journal of Heterocyclic Chemistry 48, (1), 31-37 (2011). http://dx.doi.org/10.1002/jhet.490

Jarvinen R, Silvestre AJD, Gil AM, Kallio H. "Solid state 13C CP-MAS NMR and FT-IR spectroscopic analysis of cuticular fractions of berries and suberized membranes of potato" Journal of Food Composition and Analysis 24, (3), 334-345 (2011). http://dx.doi.org/10.1016/j.jfca.2010.09.022

Kijjoa A, Santos S, Dethoup T, Manoch L, Almeida AP, Vasconcelos MH, Silva A, Gales L, Herz W. "Sartoryglabrins, Analogs of Ardeemins, from Neosartorya glabra" Natural Product Communications 6, (6), 807-812 (2011).

Li XW, Zhou CF, Lin Z, Rocha J, Lito PF, Santiago AS, Silva CM. "Titanosilicate AM-3 membrane A new potential candidate for H2 separation" Microporous and Mesoporous Materials 137, (1-3), 43-48 (2011). http://dx.doi.org/10.1016/j.micromeso.2010.08.019

Lin S, Shi L, Carrott M, Carrott PJM, Rocha J, Li MR, Zou XD. "Direct synthesis without addition of acid of Al-SBA-15 with controllable porosity and high hydrothermal stability" Microporous and Mesoporous Materials 142, (2-3), 526-534 (2011). http://dx.doi.org/10.1016/j.micromeso.2010.12.043

Menezes J, Gomes A, Silva AMS, Faustino MAF, Neves M, Tomé AC, da Silva FD, Ferreira VF, Cavaleiro JAS. "Reaction of β-Vinyl-meso-tetraphenylporphyrin with o-

Quinone Methides" Synlett 2011, (13), 1841-1844. http://dx.doi.org/10.1055/s-0030-1260947

Moujir LM, Seca AML, Araujo L, Silva AMS, Barreto MC. "A new natural spiro heterocyclic compound and the cytotoxic activity of the secondary metabolites from Juniperus brevifolia leaves" Fitoterapia 82, (2), 225-229 (2011). http://dx.doi.org/10.1016/j.fitote.2010.10.001

Moura NMM, Faustino MAF, Neves M, Duarte AC, Cavaleiro JAS. "Vilsmeier-Haack formylation of Cu(II) and Ni(II) porphyrin complexes under microwaves irradiation" Journal of Porphyrins and Phthalocyanines 15, (7-8), 652-658 (2011). http://dx.doi.org/10.1142/S1088424611003586

Neri DFM, Balcao VM, Cardoso SM, Silva AMS, Domingues MDM, Torres DPM, Rodrigues LRM, Carvalho LB, Teixeira JAC. "Characterization of galactooligosaccharides produced by β-galactosidase immobilized onto magnetized Dacron" International Dairy Journal 21, (3), 172-178 (2011). http://dx.doi.org/10.1016/j.idairyj.2010.10.009

Neves CMB, Simões MMQ, Santos I, Domingues FMJ, Neves M, Paz FAA, Silva AMS, Cavaleiro JAS. "Oxidation of caffeine with hydrogen peroxide catalyzed by metalloporphyrins" Tetrahedron Letters 52, (22), 2898-2902 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.03.139

Neves MP, Cidade H, Pinto M, Silva AMS, Gales L, Damas AM, Lima RT, Vasconcelos MH, Nascimento MDJ. "Prenylated derivatives of baicalein and 3,7-dihydroxyflavone: Synthesis and study of their effects on tumor cell lines growth, cell cycle and apoptosis" Eur J Med Chem 46, (6), 2562-74 (2011). http://dx.doi.org/10.1016/j.ejmech.2011.03.047

Oliveira CM, Ferreira ACS, De Freitas V, Silva AMS. "Oxidation mechanisms occurring in wines". Food Research International 44, (5), 1115-1126 (2011). http://dx.doi.org/10.1016/j.foodres.2011.03.050

Oliveira JR, Martins MCL, Mafra L, Gomes P. "Synthesis of an O-alkynyl-chitosan and its chemoselective conjugation with a PEG-like amino-azide through click chemistry" Carbohydrates Polymers 87, (1), 240-249 (2011). http://dx.doi.org/10.1016/j.carbpol.2011.07.043

Paixao V, Monteiro R, Andrade M, Fernandes A, Rocha J, Carvalho AP, Martins A. "Desilication of MOR zeolite: Conventional versus microwave assisted heating" Applied Catalysis A: General 402, (1-2), 59-68 (2011). http://dx.doi.org/10.1016/j.apcata.2011.05.025

Pedrosa LF, de Souza MC, Faustino MAF, Neves M, Silva AMS, Tomé AC, Ferreira VF, Cavaleiro JAS. "Porphyrin-Phosphoramidate Conjugates: Synthesis, Photostability and Singlet Oxygen Generation" Australian Journal of Chemistry, 64, (7), 939-944 (2011). http://dx.doi.org/10.1071/CH11013

Pinto D, Seca AML, Leal SB, Silva AMS, Cavaleiro JAS. "A Novel Short-Step Synthesis of New Xanthenedione Derivatives from the Cyclization of 3-Cinnamoyl-2-styrylchromones" Synlett 2011, (14), 2005-2008 (2011). http://dx.doi.org/10.1055/s-0030-1261172

Pinto ML, Mafra L, Guil JM, Pires J, Rocha J. "Adsorption and Activation of CO2 by Amine-Modified Nanoporous Materials Studied by Solid-State NMR and 13CO2 Adsorption" Chem. Mater. 23, (6), 1387-1395 (2011). http://dx.doi.org/10.1021/cm1029563

Pires SMG, De Paula R, Simões MMQ, Silva AMS, Domingues MRM, Santos I, Vargas MD, Ferreira VF, Neves M, Cavaleiro JAS. "Novel biomimetic oxidation of lapachol with H2O2 catalysed by a manganese(III) porphyrin complex" RSC Advances 1, 1195-1199 (2011). http://dx.doi.org/10.1039/C1RA00578B

Resende D, Silva EMP, Barros C, Domingues MRM, Silva AMS, Cavaleiro JAS. "Tandem mass spectrometry based investigation of cinnamylideneacetophenone derivatives: valuable tool for the differentiation of positional isomers" Rapid Communications in Mass Spectrometry 25, (20), 3185-3195 (2011). http://dx.doi.org/10.1002/rcm.5207

Rocha CM, Carrola J, Barros AS, Gil AM, Goodfellow BJ, Carreira IM, Bernardo J, Gomes A, Sousa V, Carvalho L, Duarte IF. "Metabolic Signatures of Lung Cancer in Biofluids: NMR-Based Metabonomics of Blood Plasma". J Proteome Res. 10, (9), 4314-24. http://dx.doi.org/10.1021/pr200550p

Rodrigues D, Santos CH, Rocha-Santos TAP, Gomes AM, Goodfellow BJ, Freitas AC. "Metabolic Profiling of Potential Probiotic or Synbiotic Cheeses by Nuclear Magnetic Resonance (NMR) Spectroscopy" J Agric Food Chem. 59 (9), 4955-4961 (2011). http://dx.doi.org/10.1021/jf104605r

Rodrigues JA, Barros AS, Carvalho B, Brandão T, Gil AM. "Probing beer aging chemistry by nuclear magnetic resonance and multivariate analysis" Anal Chim Acta 702,

(2), 178-87 (2011). http://dx.doi.org/10.1016/j.aca.2011.06.042

Rodrigues JA, Barros AS, Carvalho B, Brandão T, Gil AM, Ferreira ACS. "Evaluation of beer deterioration by gas chromatography-mass spectrometry/multivariate analysis: A rapid tool for assessing beer composition". J Chromatogr A. 1218, (7), 990-996 (2011). http://dx.doi.org/10.1016/j.chroma.2010.12.088

Santos CMM, Silva AMS, Filipe P, Santus R, Patterson LK, Maziere JC, Cavaleiro JAS, Morliere P. "Structure-activity relationships in hydroxy-2,3-diarylxanthone antioxidants. Fast kinetics spectroscopy as a tool to evaluate the potential for antioxidant activity in biological systems" Organic & Biomolecular Chemistry 9 (10), 3965-3974 (2011). http://dx.doi.org/10.1039/c0ob00841a

Seixas R, Silva AMS, Alkorta I, Elguero J. "An experimental NMR and computational study of 4-quinolones and related compounds" Monatshefte Fur Chemie 142, (7), 731-742 (2011). http://dx.doi.org/10.1007/s00706-011-0473-y

Siegel R, Mafra L, Rocha J. "Improving the 1H indirect dimension resolution of 2D CRAMPS NMR spectra: A simulation and experimental investigation" Solid State Nuclear Magnetic Resonance 39, (3-4), 81-87 (2011). http://dx.doi.org/10.1016/j.ssnmr.2011.04.003

Silva EMP, Silva AMS, Cavaleiro JAS. "1,6-Conjugated Addition of Nitromethane to (E)-2-Styrylchromones: A New Synthesis of Novel 2-Substituted 4-Arylpyrrole Derivatives" Synlett 2011, (18), 2740-2744 (2011). http://dx.doi.org/10.1055/s-0031-1289525

Silva P, Vieira F, Gomes AC, Ananias D, Fernandes JA, Bruno SM, Soares R, Valente AA, Rocha J, Paz FAA. "Thermal Transformation of a Layered Multifunctional Network into a Metal-Organic Framework Based on a Polymeric Organic Linker" J Am Chem Soc. 133, (38), 15120-38 (2011). http://dx.doi.org/10.1021/ja205243w

Soares-Santos PCR, Cunha-Silva L, Sousa FL, Sousa JLC, Gates PJ, Klinowski J, Trindade T, Rocha J, Cavaleiro AMV, Paz FAA, Nogueira HIS. "A new supramolecular organic-inorganic adduct: {[Eu(CH3OH)(H2O)8]2[Eu(H2O)8][PW12O40]3} · 8(C14H20O5) · 2(C28H40O10) · 6(CH3OH) · 6H2O)" Journal of Molecular Structure 989, (1-3), 80-85 (2011). http://dx.doi.org/10.1016/j.molstruc.2011.01.007

Trovatti E, Silva NHCS, Duarte IF, Rosado CF, Almeida IF, Costa P, Freire CSR, Silvestre AJD, Neto CP. "Biocellulose Membranes as Supports for Dermal Release of Lidocaine" Biomacromolecules 12, (11), 4162-4168 (2011). http://dx.doi.org/10.1021/bm201303r

Vasas A, Patonay T, Konya K, Silva AMS, Cavaleiro JAS. "The Heck Reaction of Protected Hydroxychromones: on route to Natural Products" Australian Journal of Chemistry 64, (5), 647-657 (2011). http://dx.doi.org/10.1071/CH10296

Zhang M, Vilarinho PM, Salvado IMM, Silva A. "Organic acids on the fabrication of sol-gel lead zirconate titanate fibers" Materials Research Bulletin 46, (9), 1515-1520 (2011). http://dx.doi.org/10.1016/j.materresbull.2010.05.036

Almeida AIS, Silva VLM, Silva AMS, Pinto D, Cavaleiro JAS. "Diels-Alder Reactions of (E)-2-Styrylquinolin-4(1H)-ones with N-Methylmaleimide: New Syntheses of Acridin-9(10H)-ones". Synlett 2012 (6), 889-892 (2012). http://dx.doi.org/10.1055/s-0031-1290600

Amorim R, Vilaca N, Martinho O, Reis RM, Sardo M, Rocha J, Fonseca AM, Baltazar F, Neves IC. "Zeolite Structures Loading with an Anticancer Compound As Drug Delivery Systems" J Phys Chem C, 116 (48): 25642-25650 (2012). http://dx.doi.org/10.1021/jp3093868

Bai X, Pucci A, Freitas VT, Ferreira RAS, Pinna N. "One-Step Synthesis and Optical Properties of Benzoate- and Biphenolate-Capped ZrO2 Nanoparticles" Advanced Functional Materials 22 (20): 4275-4283 (2012). http://dx.doi.org/10.1002/adfm.201200759

Batista MLS, Tome LIN, Neves C, Rocha EM, Gomes JRB, Coutinho JAP. "The Origin of the LCST on the Liquid-Liquid Equilibrium of Thiophene with Ionic Liquids" J Phys Chem B, 116 (20): 5985-5992 (2012). http://dx.doi.org/10.1021/jp303187z

Buttachon S, Chandrapatya A, Manoch L, Silva A, Gales L, Bruyere C, Kiss R, Kijjoa A. "Sartorymensin, a new indole alkaloid, and new analogues of tryptoquivaline and fiscalins produced by Neosartorya siamensis (KUFC 6349)" Tetrahedron, 68 (15): 3253-3262 (2012). http://dx.doi.org/10.1016/j.tet.2012.02.024

Cardote TAF, Barata JFB, Faustino MAF, Preuss A, Neves M, Cavaleiro JAS, Ramos CIV, Santana-Marques MGO, Roder B. "Pentafluorophenylcorrole-D-galactose conjugates". Tetrahedron Letters, 53 (47): 6388-6393 (2012). http://dx.doi.org/10.1016/j.tetlet.2012.09.038

Craveiro R, Lin Z. "The influence of Fe on the formation of titanosilicate ETS-4" Journal of Solid State Chemistry 190, 162-168 (2012). http://dx.doi.org/10.1016/j.jssc.2012.02.037

Duarte IF, Gil AM. "Metabolic signatures of cancer unveiled by NMR spectroscopy of human biofluids". Progress in Nuclear Magnetic Resonance Spectroscopy 62, 51-74 (2012). http://dx.doi.org/10.1016/j.pnmrs.2011.11.002

Figueiredo S, Gomes AC, Neves P, Amarante TR, Paz FAA, Soares R, Lopes AD, Valente AA, Pillinger M, Goncalves IS. "Synthesis, Structural Elucidation, and Application of a Pyrazolylpyridine-Molybdenum Oxide Composite as a Heterogeneous Catalyst for Olefin Epoxidation". Inorganic Chemistry 51, (15), 8629-8635 (2012). http://dx.doi.org/10.1021/ic301405r

Graca G, Diaz SO, Pinto J, Barros AS, Duarte IF, Goodfellow BJ, Galhano E, Pita C, Almeida MD, Carreira IM, Gil AM. "Can Biofluids Metabolic Profiling Help to Improve Healthcare during Pregnancy?" Spectroscopy-an International Journal 27 (5-6): 515-523 (2012). http://dx.doi.org/10.1155/2012/128367

Graca G, Goodfellow BJ, Barros AS, Diaz S, Duarte IF, Spagou K, Veselkov K, Want EJ, Lindon JC, Carreira IM, Galhano E, Pita C, Gil AM. "UPLC-MS metabolic profiling of second trimester amniotic fluid and maternal urine and comparison with NMR spectral profiling for the identification of pregnancy disorder biomarkers". Molecular Biosystems 8 (4): 1243-1254 (2012). http://dx.doi.org/10.1039/c2mb05424h

Lima C, Gomes LR, Low JN, Silva AMS, Santos L. "Elucidating the Role of Aromatic Interactions in Rotational Barriers Involving Aromatic Systems". J Org Chem. 77 (22): 10422-10426 (2012). http://dx.doi.org/10.1021/jo301629y

Mafra L, Santos SM, Siegel R, Alves I, Paz FAA, Dudenko D, Spiess HW. "Packing Interactions in Hydrated and Anhydrous Forms of the Antibiotic Ciprofloxacin: a Solid-State NMR, X-ray Diffraction, and Computer Simulation Study" J Am Chem Soc. 134 (1): 71-74 (2012). http://dx.doi.org/10.1021/ja208647n

Monteiro CJP, Pereira MM, Goncalves NPF, Carvalho CG, Neves ACB, Abreu AR, Arnaut LG, Silva AMS. "Separation and atropisomer isolation of ortho-halogenated tetraarylporphyrins by HPLC. Full characterization using 1D and 2D NMR". Journal of Porphyrins and Phthalocyanines 16, (3): 316-323 (2012). http://dx.doi.org/10.1142/S1088424612500368

Neves CMB, Simoes MMQ, Domingues FMJ, Neves M, Cavaleiro JAS. "Biomimetic Oxidation Of Carbamazepine With Hydrogen Peroxide Catalyzed By A Manganese Porphyrin". Quimica Nova 35, (7): 1477-U265 (2012). http://dx.doi.org/10.1590/S0100-40422012000700033

Nunes SC, Silva NJO, Hummer J, Ferreira RAS, Almeida P, Carlos LD, Bermudez VD. "Water-mediated structural tunability of an alkyl/siloxane hybrid: from amorphous material to lamellar structure or bilamellar superstructure". RSC Advances 2 (5): 2087-2099 (2012). http://dx.doi.org/10.1039/C2RA00702A

Oliveira JR, Martins MCL, Mafra L, Comes P. "Synthesis of an O-alkynyl-chitosan and its chemoselective conjugation with a PEG-like amino-azide through click chemistry". Carbohydrate Polymers 87 (1): 240-249 (2012). http://dx.doi.org/10.1016/j.carbpol.2011.07.043

Patoilo DT, Silva AMS, Pinto D, Santos CMM, Tome AC, Cavaleiro JAS. "Tetrahydroquinazoline-substituted chromones from Diels-Alder reaction of (E)-2-styrylchromones and pyrimidine ortho-quinodimethane". Tetrahedron Letters 53 (22): 2722-2725 (2012). http://dx.doi.org/10.1016/j.tetlet.2012.03.081

Pereira OR, Domingues MRM, Silva AMS, Cardoso SM. "Phenolic constituents of Lamium album: Focus on isoscutellarein derivatives" Food Research International 48 (1): 330-335 (2012). http://dx.doi.org/10.1016/j.foodres.2012.04.009

Pereira OR, Silva AMS, Domingues MRM, Cardoso SM. "Identification of phenolic constituents of Cytisus multiflorus". Food Chemistry 131 (2): 652-659 (2012). http://dx.doi.org/10.1016/j.foodchem.2011.09.045

Sousa RMS, Pinto DCGA, Silva MAS, Serra VV, Barros AIRNA, Faustino MAF, Neves MGPMS, Cavaleiro JAS. “Flavone–Nitrogen Heterocycle Conjugate Formation by 1,3-Dipolar Cycloadditions” Eur. J. Org. Chem, 2012: 132-143 (2012). http://dx.doi.org/10.1002/ejoc.201101185

Prozil SO, Costa EV, Evtuguin DV, Lopes LPC, Domingues MRM. "Structural characterization of polysaccharides isolated from grape stalks of Vitis vinifera L" Carbohydrate Research 356: 252-259 (2012). http://dx.doi.org/10.1016/j.carres.2012.02.001

Santos CIM, Oliveira E, Barata JFB, Faustino MAF, Cavaleiro JAS, Neves M, Lodeiro C. "Corroles as anion chemosensors: exploiting their fluorescence behaviour from solution to solid-supported devices". J Mater Chem. 22: 13811-13819 (2012). http://dx.doi.org/10.1039/C2JM31281F

Santos CMM, Silva AMS, Jeko J, Levai A. "Synthesis and structure elucidation of novel pyrazolyl-2-pyrazolines obtained by the reaction of 3-(3-aryl-3-oxopropenyl)chromen-4-ones with phenylhydrazine". Arkivoc 2012, 265-281 (2012).

Santos PSM, Santos EBH, Duarte AC. "First spectroscopic study on the structural features of dissolved organic matter isolated from rainwater in different seasons". Science of the Total Environment 426: 172-179 (2012). http://dx.doi.org/10.1016/j.scitotenv.2012.03.023

Sardo M, Siegel R, Santos SM, Rocha J, Gomes JRB, Mafra L. "Combining Multinuclear High-Resolution Solid-State MAS NMR and Computational Methods for Resonance Assignment of Glutathione Tripeptide". J Phys Chem A, 116 (25): 6711-6719 (2012). http://dx.doi.org/10.1021/jp302128r

Siegel R, Domingues E, De Sousa R, Jerome F, Morais CM, Bion N, Ferreira P, Mafra L. "Understanding the high catalytic activity of propylsulfonic acid-functionalized periodic mesoporous benzenesilicas by high-resolution H-1 solid-state NMR spectroscopy". Journal of Materials Chemistry 22: 7412-7419 (2012). http://dx.doi.org/10.1039/C2JM15015H

Silva AR, Albuquerque H, Borges S, Siegel R, Mafra L, Carvalho AP, Pires J. "Strategies for copper bis(oxazoline) immobilization onto porous silica based materials". Microporous and Mesoporous Materials, 158: 26-38 (2012). http://dx.doi.org/10.1016/j.micromeso.2012.02.044

Talhi O, Silva AMS. "Advances in C-glycosylflavonoid Research". Current Organic Chemistry, 16 (7): 859-896 (2012). http://dx.doi.org/10.2174/138527212800194791

Vilela SMF, Ananias D, Gomes AC, Valente AA, Carlos LD, Cavaleiro JAS, Rocha J, Tome JPC, Paz FAA. "Multi-functional metal-organic frameworks assembled from a tripodal organic linker". Journal of Materials Chemistry, 22 (35): 18354-18371 (2012). http://dx.doi.org/10.1039/C2JM32501B

Roca C, Chagas B, Farinha I, Freitas F, Mafra L, Aguiar F, Oliveira R, Reis MAM. “Production of yeast chitin-glucan complex from biodiesel industry byproduct”. Process Biochem. 47 (11): 1670–1675 (2012). http://dx.doi.org/10.1016/j.procbio.2012.04.004

Pinho SLC, Faneca H, Geraldes CFGC, Delville MH, Carlos LD, Rocha J. “Lanthanide-DTPA grafted silica nanoparticles as bimodal-imaging contrast agents”, Biomaterials, 33: 925-935 (2012). http://dx.doi.org/10.1016/j.biomaterials.2011.09.086

Pinho SLC, Feneca H, Geraldes CFGC, Rocha J, Carlos LD, Delville MH. “Silica nanoparticles for bimodal MRI-optical imaging via grafting of Gd3+ and Eu3+/Tb3+ complexes”, Eur. J. Inorg. Chem., 2828-2837 (2012). http://dx.doi.org/10.1002/ejic.201101110

Pinho SLC, Laurent S, Rocha J, Roch A, Delville MH, Mornet S, Carlos LD, Vander Elst L, Muller RN, Geraldes CFGC. “Relaxometric Studies of gamma-Fe2O3@SiO2 Core Shell Nanoparticles: When the Coating Matters”, J. Phys. Chem. C, 116 (3), 2285-2291 (2012). http://dx.doi.org/10.1021/jp2086413

Ananias D, Almeida Paz FA, Carlos LD, Rocha J. “Chiral microporous rare-earth silico-germanates: Synthesis, structure and photoluminescence properties”, Microporous and Mesoporous Materials, 166: 50-58 (2012). http://dx.doi.org/10.1016/j.micromeso.2012.04.032

Debasu ML, Ananias D, Pinho SLC, Geraldes CFGC, Carlos LD, Rocha J. “(Gd,Yb,Tb)PO4 up-conversion nanocrystals for bimodal luminescence-MR imaging”, Nanoscale, 4: 5154-5162 (2012). http://dx.doi.org/10.1039/C2NR31226C

Pinheiro A, Dethoup T, Bessa J, Silva AMS, Kijjoa A. “A new bicyclic sesquiterpene from the marine sponge associated fungus Emericellopsis minima”, Phytochemistry Lett. 5 (1): 68-70 (2012). http://dx.doi.org/10.1016/j.phytol.2011.10.002

Cumella J, Hernández-Folgado L, Girón R, Sánchez E, Morales P, Hurst DP, Gómez-Cañas M, Gómez-Ruiz M, Pinto DCGA, Goya P, Reggio PH, Martin MI, Fernández-Ruiz J, Silva AMS, Jagerovic N. “Chromenopyrazoles: Non-psychoactive and Selective CB1 Cannabinoid Agonists with Peripheral Antinociceptive Properties”, ChemMedChem, 7, 452-463 (2012). http://dx.doi.org/10.1002/cmdc.201100568

Soengas RG, Silva AMS. “Indium-Catalyzed Henry-Type Reaction of Aldehydes with Bromonitroalkanes”, Synlett 2012, 23, 873-876 (2012). http://dx.doi.org/10.1055/s-0031-1290617

Patinha DJS, Domingues RMA, Villaverde JJ, Silva AMS, Silva CM, Freire CSR, Pascoal Neto C, Silvestre AJD. “Lipophilic extractives from the bark of Eucalyptus grandis x globulus, a rich source of methyl morolate: Selective extraction with supercritical CO2”, Ind. Crops Prod., 43: 340-348 (2012). http://dx.doi.org/10.1016/j.indcrop.2012.06.056

Vaz PAAM, Pinto DCGA, Rocha DHA, Silva AMS, Cavaleiro JAS. “New Syntheses of 3-Aroylflavone Derivatives; Knoevenagel Condensation and Oxidation versus On-Pot Synthesis”, Synlett 23 (16): 2353-2356 (2012). http://dx.doi.org/10.1055/s-0032-1317159

Neves CMB, Simões MMQ, Domingues MRM, Santos ICMS, Neves MGPMS, Almeida Paz FA, Silva AMS, Cavaleiro JAS. “Oxidation of diclofenac catalyzed by manganese porphyrins: synthesis of novel diclofenac derivatives”, RSC Advances, 2: 7427–7438 (2012). http://dx.doi.org/10.1039/C2RA20801F

Neves MP, Cravo S, Lima RT, Vasconcelos MH, São José Nascimento M, Silva AMS, Pinto M, Cidade H, Correia AG. “Solid-phase synthesis of 2’-hydroxychalcones. Effects on cell growth inhibition, cell cycle and apoptosis of human tumor cell lines”, Bioorg. Med. Chem., 20 (1): 25-33 (2012). http://dx.doi.org/10.1016/j.bmc.2011.11.042

Neves MP, Lima RT, Choosang K, Pakkong P, São José Nascimento M, Vasconcelos MH, Pinto M, Silva AMS, Cidade H. “Synthesis of a Natural Chalcone and Its Prenyl Analogs – Evaluation of Tumor Cell Growth-Inhibitory Activities, and Effects on Cell Cycle and Apoptosis”, Chem. & Biodiversity 9 (6): 1133-1143 (2012). http://dx.doi.org/10.1002/cbdv.201100190

Costa DCS, Gomes MC, Faustino MAF, Neves MGPMS, Cunha A, Cavaleiro JAS, Almeida A, Tomé JPC. “Comparative photodynamic inactivation studies of antibiotic resistant bacteria by pyridinium porphyrin and chlorin derivatives”, Photochem. Photobiol. Sci., 11 (12): 1905-1913 (2012). http://dx.doi.org/10.1039/c2pp25113b

Pereira JB, Carvalho EFA, Faustino MAF, Neves MGPMS, Cavaleiro JAS, Cunha A, Almeida A, Tomé JPC. “Phthalocyanine thio-pyridinium derivatives as antibacterial photosensitizers” Photochem. Photobiol. 88 (3), 537-547 (2012). http://dx.doi.org/10.1111/j.1751-1097.2012.01113.x

Menezes JCJMDS, Pereira AMVM, Neves MGPMS, Silva MAS, Santos SM, Martinez, ST, Silva BV, Pinto AC, Cavaleiro JAS. “Synthesis of porphyrin indolin-2-one conjugates via palladium-catalyzed amination reactions”, Tetrahedron, 68 (39): 8330-8339 (2012). http://dx.doi.org/10.1016/j.tet.2012.07.024

Moura NMM, Faustino MAF, Neves MGPMS, Paz FAA, Silva AMS, Tomé AC, Cavaleiro JAS. “A new synthetic approach to benzoporphyrins and Kröhnke type porphyrin-2-ylpyridines”, Chem. Commun., 48: 6142–6144 (2012). http://dx.doi.org/10.1039/C2CC30727H

Moura NMM, Faustino MAF, Neves MGPMS, Tomé AC, Rakib EM, Hannioui A, Mojahidi S, Hackbarth S, Röder B, Paz FAA, Silva AMS, Cavaleiro JAS. “Novel pyrazoline and pyrazole porphyrin derivatives: synthesis and photophysical properties”, Tetrahedron, 68 (39): 8181-8193 (2012). http://dx.doi.org/10.1016/j.tet.2012.07.072

Silva EMP, Ramos CIV, Pereira PMR, Giuntini F, Faustino MAF, Tomé JPC, Tomé AC, Silva AMS, Santana-Marques MG, Neves MGPMS, Cavaleiro JAS. “Cationic β-vinyl substituted meso-tetraphenylporphyrins: synthesis and non-covalent interactions with a short poly(dGdC) duplex”, J. Porphyrins Phthalocyanines, 16, 101–113 (2012). http://dx.doi.org/10.1142/S1088424611004373

Silva S, Pereira PMR, Silva P, Paz FAA, Faustino MAF, Cavaleiro JAS, Tomé JPC. “Porphyrin and phthalocyanine glycodendritic conjugates: synthesis, photophysical and photochemical properties”, Chem. Commun., 48, 3608–3610 (2012). http://dx.doi.org/10.1039/C2CC17561D

CNC – Universidade de Coimbra

Book Chapters

J. G. Jones “Direct and indirect pathways of hepatic glycogen synthesis in normal and in insulin resistant states”, Chapter 6, in Advances in Medicine and Biology - Volume 13, edited by Leon V. Berhardt. 2010 Nova Science Publishers Inc. ISBN: 9781617614385.

Carlos F.G.C. Geraldes “The Rare Earth Elements: Fundamentals and Applications”, in Encyclopedia of Inorganic and Bioinorganic Chemistry, edited by David A. Atwood. John Wiley & Sons, Ltd, Chichester, UK, pp. 501-520 (2012). ISBN: 978-1-1199-5097-4

Carla P. Fonseca , Liliana P. Montezinho and M. Margarida C. A. Castro “Li+ in bipolar disorder – possible mechanisms of its pharmacological mode of action” in Bipolar Disorder – A Portrait of a Complex Mood Disorder, Intech Ed., Chapter 4, pg. 57-98 (2012).

Joop A. Peters, Kristina Djanashvili, Carlos F.G.C. Geraldes, Carlos Platas-Iglesias “Structure, Dynamics and Computational Studies of Lanthanide Based Contrast Agents” in The Chemistry of Contrast Agents in Medical Magnetic Resonance Imaging, A.E. Merbach, Ed., John Wiley and Sons, 2.nd edition, in press. ISBN: 978-1-119-99176-2

Ivan Viegas, Rui de Albuquerque Carvalho, Miguel Ângelo Pardal and John Griffith Jones “Advances and Applications of Tracer Measurements of Carbohydrate Metabolism” in Fish, New Advances and Contributions to Fish Biology, Hakan Türker (Ed.), ISBN: 978-953-51-0909-9

A.F. Soares, John G. Jones “Galactose and galactose tracers in metabolic studies”, in Food and Nutritional Components Chapter 37 in Focus, Royal Society of Chemistry Publishers (2012). ISBN :9781849733700

Scientific Papers

Nacira Darghal, Arlette Garnier-Suillerot, Nadia Bouchemal, Gabriel Grasc, Carlos F.G. C. Geraldes, Milena Salerno “Accumulation of Eu3+ Chelates in Cells Expressing or not P-Glycoprotein: Implications for Blood Brain Barrier Crossing” J. Inorg. Biochem., 104, 47-54 (2010). http://dx.doi.org/10.1016/j.jinorgbio.2009.09.026

Giovannia A. Pereira, Joop A. Peters, Filipe A. Paz, João Rocha and Carlos F.G.C. Geraldes “Evaluation of [Ln(H2cmp)(H2O)] Metal Organic Framework Materials for Potential Application as MRI Contrast Agents” Inorganic Chemistry, 49, 2969–2974 (2010). http://dx.doi.org/10.1021/ic9025014

Carlos F.G.C. Geraldes, Kristina Djanashvili, Joop A. Peters “Glycoconjugate probes and targets for molecular imaging using MRI” Future Medicinal Chem., 2, 409–425 (2010). http://dx.doi.org/10.4155/fmc.09.157

M. Paula C. Campello, Sara Lacerda, Isabel C. Santos, Giovannia A. Pereira, Carlos F.G.C. Geraldes, Jan Kotek, Petr Hermann, Jakub Vaněk, Přemysl Lubal, Vojtěch Kubíček, Éva Tóth and Isabel Santos “Lanthanide(iii) Complexes of 4,10-Bis(phosphonomethyl)-1,4,7,10-tetraazacyclo-dodecane-1,7- diacetic acid (trans-H6do2a2p) in Solution and in the Solid State: Structural Studies Along the Series” Chem. Eur. J., 28, 8446-8465 (2010). http://dx.doi.org/10.1002/chem.201000320

Sonia L. C. Pinho, Giovannia A. Pereira, Pierre Voisin, Jinane Kassem, Véronique Bouchaud, Laetitia Etienne, Joop A. Peters, Luis Carlos, Stéphane Mornet, Carlos F.G.C. Geraldes, João Rocha, Marie-Hélène Delville “Fine tuning of the relaxometry of γ-Fe2O3 nanoparticles by tweaking the thickness of the silica coating” ACS Nano, 4, 5339–5349 (2010). http://dx.doi.org/10.1021/nn101129r

Marta Passadouro, Ana M. Metelo, Alice S. Melão, Joana R. Pedro, Henrique Faneca, Eugénia Carvalho, M. Margarida C.A. Castro “Study of the insulinomimetic capacity of the VO(dmpp)2 complex” J. Inorg. Biochem., 104, 987-992 (2010). http://dx.doi.org/10.1016/j.jinorgbio.2010.05.004

Cristina Barosa, Manuela Almeida, M Madalena Caldeira, Filipe Gomes, John G. Jones “Contribution of proteolytic and metabolic sources to hepatic glutamine by 2H NMR analysis of urinary phenylacetylglutamine 2H-enrichment from 2H2O” Metab. Eng. 12, 53-61 (2010). http://dx.doi.org/10.1016/j.ymben.2009.08.009

Soares, A.F.,Veiga, F.J., Carvalho, R.A. and Jones, J.G. “Effects of galactose on direct and indirect pathway estimates of hepatic glycogen synthesis” Metab. Eng. 12, 552-560 (2010). http://dx.doi.org/10.1016/j.ymben.2010.08.002

Silvia Chaves, Ana C. Mendonça, Sérgio M. Marques, Maria I.M. Prata, Ana C. Santos, André F. Martins, Carlos F.G.C. Geraldes, M. Amélia Santos “A Gallium Complex with a New Tripodal Tris-Hydroxypyridinone for Potential Nuclear Diagnostic Imaging: Solution and in vivo Studies of 67Ga-Labeled Species”, J. Inorg. Biochem., 105, 31-38 (2011). http://dx.doi.org/j.jinorgbio.2010.09.012

André Fontes, M. Isabel M. Prata, Carlos F. G. C. Geraldes, João P. André “Ga(III) chelates of amphiphilic DOTA-based ligands: synthetic route and in vitro and in vivo studies” Nucl. Med. Biology, 38, 363-370 (2011). http://dx.doi.org/10.1016/j.nucmedbio.2010.10.003

João M. C. Teixeira, David M. Dias, F. Javier Cañada, José A. Martins, João P. André, Jesús Jiménez-Barbero, and Carlos F. G. C. Geraldes "The Interaction of La3+ Complexes of DOTA/DTPA-Glycoconjugates with the RCA120 lectin: A Saturation Transfer Difference (STD) NMR Spectroscopic Study" J. Biol. Inorg. Chem., 16, 725-734 (2011). http://dx.doi.org/10.1007/s00775-011-0773-z

Oliveira P. F., Alves M. G.; Rato L.; Silva, J., Sa, R. Barros, A., Sousa, M., Carvalho, R.A, Cavaco, J.E., Socorro, S. "Influence of 5α-dihydrotestosterone and 17β-estradiol on human Sertoli cells metabolism" Journal of Andrology, 34, E612-E620 (2011) http://dx.doi.org/10.1111/j.1365-2605.2011.01205.x

M. Fellner, P. Riß, N. Loktionova, K. Zhernosekov, O. Thews, C.F.G.C. Geraldes, Z. Kovacs, I. Lukeš, F. Rösch "Comparison of different phosphorus-containing ligands complexing 68Ga for PET-imaging of bone metabolism", Radiochimica Acta, 99, 43-51 (2011). http://dx.doi.org/10.1524/ract.2011.1791

Sara Figueiredo, João Nuno Moreira, Carlos F.G.C. Geraldes, Silvio Aime, Enzo Terreno "Supramolecular Protamine/Gd-loaded Liposomes Adducts as Relaxometric Protease Responsive Probes", Bioorg. Medicinal Chem., 19, 1131-1135 (2011). http://dx.doi.org/10.1016/j.bmc.2010.07.057

João P. Monteiro, André F. Martins, Marlene Lúcio, Salette Reis, Carlos F.G.C Geraldes, Paulo J. Oliveira and Amália S. Jurado "Interaction of carbonylcyanide p-trifluoromethoxyphenylhydrazone (FCCP) with lipid membrane systems: a biophysical approach with relevance to mitochondrial uncoupling", J. Bioenerg. Biomembranes 43, 287–298 (2011). http://dx.doi.org/10.1007/s10863-011-9359-2

David M. Dias, João M.C. Teixeira, Ilya Kuprov, Elizabeth J. New , David Parker and Carlos F.G.C. Geraldes "Enantioselective binding of a lanthanide(III) complex to human serum albumin studied by 1H STD NMR techniques", Org. Biomol. Chem., 9, 5047-5050 (2011). http://dx.doi.org/10.1039/C1OB05524K

João P. Monteiro, André F. Martins, Marlene Lúcio, Salette Reis, Teresa J. Pinheiro, Carlos F.G.C Geraldes, Paulo J. Oliveira and Amália S. Jurado "Nimesulide interaction with membrane model systems: are membrane physical effects involved in nimesulide mitochondrial activity?", Toxicology in Vitro, 25, 1215-1223 (2011). http://dx.doi.org/10.1016/j.tiv.2011.05.014

Sara Figueiredo, João Nuno Moreira, Carlos F.G.C. Geraldes, Silvia Rizzitelli, Silvio Aime, Enzo Terreno "Yeast Cell Wall Particles: a promising class of nature-inspired microcarriers formultimodal imaging", Chem. Comm., 47, 10635-10637 (2011). http://dx.doi.org/10.1039/C1CC14019A

Viegas I, Mendes VM, Leston S, Jarak I, Carvalho RA, Pardal MA, Manadas B, Jones JG "Analysis of glucose metabolism in farmed european sea bass (Dicentrarchus labrax L.) using deuterated water", Comp Biochem Physiol A Mol Integr Physiol., 160, 341-7, (2011). http://dx.doi.org/10.1016/j.cbpa.2011.06.029

Kacerovsky M, Jones, JG, Schmid, AI, Barosa, C, Lettner A, Kacerovsky-Bielesz G, Szendroedi J, Chmelik M, Nowotny P, Chandramouli V, Wolzt M, Roden M. "Postprandial and fasting hepatic glucose fluxes in longstanding type 1 diabetes", Diabetes, 60, 1752-1758 (2011). http://dx.doi.org/10.2337/db10-1001

Silva AP, Martins F, Jones JG, Carvalho RA "2H2O Incorporation Into Hepatic Acetyl-CoA and De novo Lipogenesis as Measured by Krebs Cycle-Mediated 2H-Enrichment of Glutamate and Glutamine", Magn. Reson. Med. 66, (6) 1526-1530 (2011). http://dx.doi.org/10.1002/mrm.22955

Nunes PM, Jones JG, Rolo AP, Palmeira CM, Carvalho RA, "Ursodeoxycholic acid treatment of hepatic steatosis: a 13C NMR metabolic study". NMR in Biomedicine 24:1145-1158 (2011). http://dx.doi.org/10.1002/nbm.1672

Basu R, Barosa C, Basu A, Pattan V, Saad A, Jones J, Rizza R. "Transaldolase exchange and its effects on measurements of gluconeogenesis in humans". Am. J. Physiol. Endocrinol Metab 300, E296-E303 (2011). http://dx.doi.org/10.1152/ajpendo.00403.2010

Ramos ML, Justino LL, Burrows HD "Structural considerations and reactivity of peroxocomplexes of V(V), Mo(VI) and W(VI)", Dalton Trans. 40 4374-4383 (2011). http://dx.doi.org/10.1039/c0dt01095b

Licínia LG Justino, M. Luísa Ramos, Matti Knaapila, Ana T. Marques, Christof J Kudla, Ullrich Scherf, László Almásy, Ralf Schweins, Hugh D. Burrows and Andrew P. Monkman "Gel Formation and Interpolymer Alkyl Chain Interactions with Poly(9,9-dioctylfluorene-2,7-diyl) (PFO) in Toluene Solution: Results from NMR, SANS, DFT, and Semiempirical Calculations and Their Implications for PFO

beta-Phase Formation", Macromolecules 44 334-343 (2011). http://dx.doi.org/10.1021/ma102235r

Luísa Ramos M, Justino LL, Branco A, Duarte CM, Abreu PE, Fonseca SM, Burrows HD, "NMR, DFT and Luminescence Studies of the Complexation of Zn(II) with 8-hydroxyquinoline-5-sulfonate", Dalton Trans. 40 11732-11741, (2011). http://dx.doi.org/10.1039/c1dt10978b

Maia J, Carvalho RA, Coelho JFJ, Simões PN, Gil MH "Insight on the periodate oxidation of dextran and its structural vicissitudes", Polymer, 52, 258-265, (2011). http://dx.doi.org/10.1016/j.polymer.2010.11.058

Carvalho RA, Correia HA, Valente AJ, Soderman O, Nilsson M "The effect of the head-group spacer length of 12-s-12 gemini surfactants in the host-guest association with beta-cyclodextrin", J. Colloid Interface Sci., 354, 725-732, (2011). http://dx.doi.org/10.1016/j.jcis.2010.11.024

Pereira RF, Tapia MJ; Valente AJ, Evans RC, Burrows HD, Carvalho RA. "On the flocculation and re-dissolution of trivalent lanthanide metal ions by sodium dodecyl sulfate in aqueous solutions", J. Colloid Interface Sci., 354, 670-676, (2011). http://dx.doi.org/10.1016/j.jcis.2010.10.063

Alves MG, Soares AF, Carvalho RA, Oliveira PJ "Sodium hydrosulfide improves the protective potential of the cardioplegic histidine buffer solution", Eur. J. Pharmacology, 654, 60-67, (2011). http://dx.doi.org/10.1016/j.ejphar.2010.12.010

Alves TC, Befroy DE, Kibbey RG, Kahn M, Codella R, Carvalho RA, Falk Petersen K, Shulman GI "Regulation of Hepatic Fat and Glucose Oxidation in Rats with Lipid-Induced Hepatic Insulin Resistance", Hepatology, 53, 1175-1181, (2011). http://dx.doi.org/10.1002/hep.24170

Costa VM, Carvalho F, Bastos ML, Carvalho RA, Carvalho M, Remião F "Contribution of Catecholamine Reactive Intermediates and Oxidative Stress to the Pathologic Features of Heart Diseases", Current Medicinal Chemistry, 18, 2272-2314 (2011). http://dx.doi.org/0929-8673/11

Pereira SL, Ramalho-Santos J, Branco AF, Sardão VA, Oliveira PJ, Carvalho RA "Metabolic Remodeling During H9c2 Myoblast Differentiation: Relevance for In Vitro Toxicity Studies", Cardiovascular Toxicology, 11, 180-190, (2011). http://dx.doi.org/10.1007/s12012-011-9112-4

Woitiski CB, Sarmento B, Carvalho RA, Neufeld RJ, Veiga F "Facilitated nanoscale delivery of insulin across intestinal membrane models" Int. J. Pharm., 412 (1-2), 123-131, (2011). http://dx.doi.org/10.1016/j.ijpharm.2011.04.003

Valente AJM, Ribeiro ACF, Marigese RBBJ, Carvalho RA, Esteso MA, Lobo VMM "Transport properties of aqueous solutions of calcium lactate in the absence and presence of beta-cyclodextrin", Journal of Molecular Liquids, 161, 125-131, (2011). http://dx.doi.org/10.1016/j.molliq.2011.05.004

Lopes G, Alves MG, Carvalho RA, Luvoni GC, Rocha A "DNA fragmentation in canine oocytes after in vitro maturation in TCM-199 medium supplemented with different proteins", Theriogenology 76 (7), 1304-1312, (2011). http://dx.doi.org/10.1016/j.theriogenology.2011.05.037

Alves MG, Oliveira PJ, Carvalho RA "Substrate selection in hearts subjected to ischemia/reperfusion: role of cardioplegic solutions and gender", NMR in Biomedicine, 24, 1029-1037, (2011). http://dx.doi.org/10.1002/nbm.1640

Almeida JA, Faneca H, Carvalho RA, Marques EF, Pais AA "Dicationic alkylammonium bromide gemini surfactants. Membrane perturbation and skin irritation"PLoSOne, 6 e26965 (2011). http://dx.doi.org/10.1371/journal.pone.0026965

Alves MG, Machado NG, Sardão VA, Carvalho RA, Oliveira PJ "Anti-Apoptotic Protection Afforded by Cardioplegic Celsior and Histidine Buffer Solutions to Hearts Subjected to Ischemia and Ischemia/Reperfusion", J. Cell Biochem, 112, 3872-3881, (2011). http://dx.doi.org/10.1002/jcb.23320

Alves MG, Gartner A, Pereira T., Amorim I., Carvalho RA, Socorro S, Oliveira PF, Mauricio AC "Evidence of metabolic switch during human mesenchymal stem cells differentiation in neural-like cells", Eur. J. Clinical Investigation, 41, 9-9, (2011). (Meeting Abstract)

Coreta-Gomes FM, Vaz WL, Wasielewski E, Geraldes CF, Moreno MJ. "Quantification of cholesterol solubilized in bile salt micellar aqueous solutions using (13)C nuclear magnetic resonance", Anal Biochem. 427 (1): 41-8. http://dx.doi.org/10.1016/j.ab.2012.04.028

Marques AT, Burrows HD, Seixas de Melo JS, Valente AJ, Justino LL, Scherf U, Fron E, Rocha S, Hofkens J, Snedden EW, Monkman AP. "Spectroscopic properties,

excitation, and electron transfer in an anionic water-soluble poly(fluorene-alt-phenylene)-perylenediimide copolymer", J. Phys. Chem. B., 116 (25): 7548-7559 (2012). http://dx.doi.org/10.1021/jp3000703

Burrows HD, Costa D, Ramos ML, Miguel Mda G, Teixeira MH, Pais AA, Valente AJ, Bastos M, Bai G. "Does cation dehydration drive the binding of metal ions to polyelectrolytes in water? What we can learn from the behaviour of aluminium(III) and chromium(III)" Phys. Chem. Chem. Phys., 14 (22): 7950-7953 (2012). http://dx.doi.org/10.1039/c2cp40480j

Ramos ML, Justino LL, Salvador AI, de Sousa AR, Abreu PE, Fonseca SM, Burrows HD. "NMR, DFT and luminescence studies of the complexation of Al(III) with 8-hydroxyquinoline-5-sulfonate" Dalton Trans., 41 (40): 12478–12489 (2012). http://dx.doi.org/10.1039/C2DT31381B

Maria TMR, Castro RAE, Silva MR, Ramos ML, Justino LLG, Burrows HD, Canotilho J, Eusébio MES. "Polymorphism and melt crystallisation of racemic betaxolol, a β-adrenergic antagonist drug", J. Therm. Anal. Calorim. Nov. (2012). http://dx.doi.org/10.1007/s10973-012-2765-9

Ramos ML, Justino LLG, Branco A, Fonseca SM, Burrows HD. "Theoretical and experimental insights into the complexation of 8-hydroxyquinoline-5-sulfonate with divalent ions of Group 12 metals" Polyhedron, in press (2012). http://dx.doi.org/10.1016/j.poly.2012.07.074

Jarmelo S, Marques DA, Simões PN, Carvalho RA, Batista CM, Araujo-Andrade C, Gil MH, Fausto R. "Experimental (IR/Raman and 1H/13C NMR) and theoretical (DFT) studies of the preferential conformations adopted by L-lactic acid oligomers and poly(L-lactic acid) homopolymer", J Phys Chem B. 116 (1) :9-21 (2012). http://dx.doi.org/10.1021/jp205033c

Bertini I, Calderone V, Cerofolini L, Fragai M, Geraldes CF, Hermann P, Luchinat C, Parigi G, Teixeira JM. "The catalytic domain of MMP-1 studied through tagged lanthanides", FEBS Lett. 586 (5): 557-67 (2012). http://dx.doi.org/10.1016/j.febslet.2011.09.020

Pereira GA, Peters JA, Terreno E, Delli Castelli D, Aime S, Laurent S, Vander Elst L, Muller RN, Geraldes CFGC "Supramolecular Adducts of Negatively Charged Lanthanide(III) DOTP Chelates and Cyclodextrins Functionalized with Ammonium Groups : Mass Spectrometry and Nuclear Magnetic Resonance Studies", Eur. J. Inorg. Chem., 2012: 2087-98 (2012). http://dx.doi.org/10.1002/ejic.201101201

Delgado TC, Barosa C, Nunes PM, Cerdán S, Geraldes CF, Jones JG. "Resolving the sources of plasma glucose excursions following a glucose tolerance test in the rat with deuterated water and [U-13C] glucose", PLoS One, 7 (3): e34042 (2012). http://dx.doi.org/10.1371/journal.pone.0034042

Delgado TC, Barosa C, Nunes PM, Scott DK, O'Doherty RM, Cerdán S, Geraldes CF, Jones JG. "Effect of cyclosporine A on hepatic carbohydrate metabolism and hepatic gene expression in rat", Expert Opin Drug Metab Toxicol. 8 (10): 1223-30 (2012). http://dx.doi.org/10.1517/17425255.2012.709500

Martins AF, Riss PJ, Prata MIM, Coarasa AA, Rodrigues SPJ, Burchardt C, Geraldes CFGC, Kroll C, Roesch F. "Spectroscopic, radiochemical, and theoretical studies of the Ga3+-N-2-hydroxyethylpiperazine-N'-2-ethanesulfonic acid (HEPES buffer) system: Evidence for the formation of GaIII HEPES complexes in 68Ga labeling reactions" Contrast Media and Molecular Imaging, in press (2012).

Figueiredo S, Cutrin JC, Rizzitelli S, De Luca E, Moreira JN, Geraldes CF, Aime S, Terreno E. "MRI Tracking of Macrophages Labeled with Glucan Particles Entrapping a Water Insoluble Paramagnetic Gd-Based Agent", Mol Imaging Biol. Nov (2012). http://dx.doi.org/10.1007/s11307-012-0603-x

Metelo AM, Pérez-Carro R, Castro MM, López-Larrubia P. "VO(dmpp)2 normalizes pre-diabetic parameters as assessed by in vivo magnetic resonance imaging and spectroscopy" J Inorg Biochem. 115: 44-49 (2012). http://dx.doi.org/10.1016/j.jinorgbio.2012.06.001

Soares AF, Carvalho RA, Veiga FJ, Alves MG, Martins FO, Viegas I, González JD, Metón I, Baanante IV, Jones JG. "Restoration of direct pathway glycogen synthesis flux in the STZ-diabetes rat model by insulin administration" Am J Physiol Endocrinol Metab. 303 (7): E875-85 (2012). http://dx.doi.org/10.1152/ajpendo.00161.2012

Viegas I, Rito J, Jarak I, Leston S, Carvalho RA, Metón I, Pardal MA, Baanante IV, Jones JG. "Hepatic glycogen synthesis in farmed European seabass (Dicentrarchus labrax L.) is dominated by indirect pathway fluxes", Comp Biochem Physiol A Mol Integr Physiol. 163 (1): 22-29 (2012). http://dx.doi.org/10.1016/j.cbpa.2012.04.023

Reis CP, Neufeld R, Veiga F, Figueiredo IV, Jones J, Soares AF, Nunes P, Damgé C, Carvalho RA. "Effects of an oral insulin nanoparticle administration on hepatic glucose metabolism assessed by ^{13}C and ^{2}H isotopomer analysis" J Microencapsul. 29 (2): 167-76 (2012). http://dx.doi.org/10.3109/02652048.2011.638992

González JD, Caballero A, Viegas I, Metón I, Jones JG, Barra J, Fernández F, Baanante IV. "Effects of alanine aminotransferase inhibition on the intermediary metabolism in Sparus aurata through dietary amino-oxyacetate supplementation", Br J Nutr. 107 (12): 1747-56 (2012). http://dx.doi.org/10.1017/S000711451100496X

Barosa C, Silva C, Fagulha A, Barros L, Caldeira MM, Carvalheiro M, Jones JG. "Sources of hepatic glycogen synthesis following a milk-containing breakfast meal in healthy subjects" Metabolism, 61 (2): 250-254 (2012). http://dx.doi.org/10.1016/j.metabol.2011.06.022

Alves TC, Jarak I, Carvalho RA. "NMR methodologies for studying mitochondrial bioenergetics" Methods Mol Biol. 810: 281-309 (2012). http://dx.doi.org/10.1007/978-1-61779-382-0_18

Delgado TC, Martins FO, Carvalho F, Gonçalves A, Scott DK, O'Doherty RM, Macedo MP, Jones JG. "2H-enrichment distribution of hepatic glycogen from 2H2O reveals the contribution of dietary fructose to glycogen synthesis", Am J Physiol Endocrinol Metab. [Epub ahead of print] (2012).

Barosa C, Jones JG, Rizza R, Basu A, Basu R. "Acetaminophen glucuronide and plasma glucose report identical estimates of gluconeogenesis and glycogenolysis for healthy and prediabetic subjects using the deuterated water method" Magn Reson Med. (2012). http://dx.doi.org/10.1002/mrm.24485

Duarte JM, Ferreira SG, Carvalho RA, Cunha RA, Köfalvi A. "CB_1 receptor activation inhibits neuronal and astrocytic intermediary metabolism in the rat hippocampus" Neurochem Int. 60 (1): 1-8 (2012). http://dx.doi.org/10.1016/j.neuint.2011.10.019

Oliveira PF, Alves MG, Rato L, Laurentino S, Silva J, Sá R, Barros A, Sousa M, Carvalho RA, Cavaco JE, Socorro S. "Effect of insulin deprivation on metabolism and metabolism-associated gene transcript levels of in vitro cultured human Sertoli cells" Biochim Biophys Acta, 1820 (2): 84-9 (2012). http://dx.doi.org/10.1016/j.bbagen.2011.11.006

Rato L, Alves MG, Socorro S, Carvalho RA, Cavaco JE, Oliveira PF. "Metabolic modulation induced by oestradiol and DHT in immature rat Sertoli cells cultured in vitro" Biosci Rep. 32 (1): 61-9 (2012). http://dx.doi.org/10.1042/BSR20110030

Loureiro R, Tavares LC, Vega-Naredo I, Erickson JR, Holy J, Perkins EL, Carvalho RA, Oliveira PJ. "Bioenergetic remodeling controls self-renewal potential during differentiation of P19 embryonal carcinoma stem cells" European Journal of Clinical Investigation, 42: 75 (2012).

Woitiski CB, Neufeld RJ, Soares AF, Figueiredo IV, Veiga FJ, Carvalho RA. "Evaluation of hepatic glucose metabolism via gluconeogenesis and glycogenolysis after oral administration of insulin nanoparticles" Drug Dev Ind Pharm. 38 (12): 1441-50 (2012). http://dx.doi.org/10.3109/03639045.2011.653789

Vega-Naredo I, Loureiro R, Tavares LC, Branco AF, Burgeiro A, Erickson JR, Holy J, Perkins EL, Carvalho RA, Oliveira PJ. "Mitochondrial behavior on cancer stem cells and differentiated cancer cells: A key element for metabolic remodeling and regulation of chemoresistance" Biochem. Biophys. Acta –Bioenergetics, 1817, S123-S124 (2012). http://dx.doi.org/10.1016/j.bbabio.2012.06.332

Alves MG, Oliveira PF, Martins FO, Oliveira PJ, Carvalho RA. "Gender-dependent metabolic remodeling during heart preservation in cardioplegic celsior and histidine buffer solution" J Cardiovasc Pharmacol. 59 (2): 151-7 (2012). http://dx.doi.org/10.1097/FJC.0b013e3182391d17

Varela C, Tavares da Silva EJ, Amaral C, Correia da Silva G, Baptista T, Alcaro S, Costa G, Carvalho RA, Teixeira NA, Roleira FM. "New structure-activity relationships of A- and D-ring modified steroidal aromatase inhibitors: design, synthesis, and biochemical evaluation" J Med Chem., 55 (8): 3992-4002 (2012). http://dx.doi.org/10.1021/jm300262w

Duarte JM, Agostinho PM, Carvalho RA, Cunha RA. "Caffeine consumption prevents diabetes-induced memory impairment and synaptotoxicity in the hippocampus of NONcZNO10/LTJ mice" PLoS One, 7 (4): e21899 (2012). http://dx.doi.org/10.1371/journal.pone.0021899

Carvalho RA. "Cardiac TCA cycle kinetics by C-13-NMR isotopomer analysis - a basic perspective for a clinical use" Eur. J. Clinical Investigation, 42, 71-72 (2012).

Abreu CMR, Mendonca PV, Serra AC, Coelho JFJ, Popov AV, Gryn'ova G, Coote ML, Guliashvili T. "Reversible

Addition–Fragmentation Chain Transfer Polymerization of Vinyl Chloride" Macromolecules, 45 (5): 2200-2208 (2012). http://dx.doi.org/10.1021/ma300064j

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Book Chapters

Alves MJ, Azoia NG, "Stereochemistry Research Trends" in Stereochemistry Research Trends, Editor M.A. Horvat and J.H. Golob, Nova Science Publishers, 2010.

Gonçalves MST, 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.

Scientific Papers

de Assunção LR, Marinho ER, Proença FP "Guanidine: studies on the reaction with ethyl N-(2-amino-1,2-dicyanovinyl)formimidate" Arkivoc, 2010 (v), 82-91. ISSN 1551-7012.

Paiva MC, Xu W, Proença MF, Novais RM, Lægsgaard E, Besenbacher F. "Unzipping of functionalized multiwall carbon nanotubes induced by STM" Nano Letters, 10 (5): 1764-1768 (2010). http://dx.doi.org/10.1021/nl100240n

Proença MF, Costa M. "One-pot approach to the synthesis of novel 12H-chromeno[2′,3′:4,5]imidazo[1,2-a] pyridines in aqueous media" Tetrahedron 66 (25): 4542-4550. http://dx.doi.org/10.1016/j.tet.2010.04.059

Marinho E, Araújo R, Proença F "The reaction of anthranilonitrile and triethylorthoformate revisited: formation of dimeric and trimeric species" Tetrahedron, 66 (45), 8681-8689 (2010). http://dx.doi.org/10.1016/j.tet.2010.09.013

Dias AM, Cabral IM, Vila-Chã AS, Cunha DP, Senhorães N, Nobre SM, Sousa CE, Proença MF "A facile one-pot synthesis of 3-imidazolyl 1,2,4-triazoles and 1,2,4-oxadiazolones" Synlett 2010 (18): 2792-2796 (2010). http://dx.doi.org/10.1055/s-0030-1258820

Bacelar AH, Carvalho MA, Proença MF. "Synthesis and in Vitro Evaluation of Substituted Pyrimido[5,4-d]pyrimidines as a Novel Class of Antimycobacterium tuberculosis agents" Eur. J. Med. Chem., 45 (7): 3234-3239 (2010). http://dx.doi.org/10.1016/j.ejmech.2010.03.047

Areias FM, Brea J, Gregori-Puigjané E, Zaki ME, Carvalho MA, Domínguez E, Gutiérrez-de-Terán H, Proença MF, Loza MI, Mestres J. "In silico directed chemical probing of the adenosine receptor family" Bioorg. Med Chem., 18 (9): 3043-3052 (2010). http://dx.doi.org/10.1016/j.bmc.2010.03.048

Oliveira MM, Carvalho LHM, Peixoto FP, Oliveira-Campos AMF, Reis A, Domingues P, Domingues MRM. "Cleavages of photochromic compounds derived from heterocycles under Electrospray Tandem Mass Spectrometry: Study of the influence of the heteroatom in fragmentation mechanisms", Rapid Communications in Mass Spectrometry, 24 (14): 2171-2174 (2010). http://dx.doi.org/10.1002/rcm.4616

Alves MJ, Duarte VCM, Faustino H, Fortes AG "Diastereo-controled Diels-Alder Cycloadditions of Erythrose Benzylidene-Acetal 1,3-Butadienes by 4-Substituted-1,2,4-triazoline-3,5-dione. Evidence for the Stereoelectronic Effects on the Dienes" Tetrahedron: Asymmetry, 21 (15): 1817-1820 (2010). http://dx.doi.org/10.1016/j.tetasy.2010.05.001

Calhelha RC, Queiroz M-JRP "Synthesis of new thieno[3,2-b]pyridine derivatives by palladium-catalyzed couplings and intramolecular cyclizations" Tetrahedron Lett. 51 (2): 281-283 (2010). http://dx.doi.org/10.1016/j.tetlet.2009.10.138

Silva JP, Machado VA, Calhelha RC, Queiroz M-JRP, Coutinho OP "Di(hetero)arylamines in the benzo[b]thiophene series as novel potent antioxidants" Drug Discov Ther., 4 (4), 246-256 (2010).

Queiroz MJ, Calhelha RC, Vale-Silva LA, Pinto E, Lima RT, Vasconcelos MH. "Efficient synthesis of 6-(hetero)arylthieno[3,2-b]pyridines by Suzuki-Miyaura coupling. Evaluation of growth inhibition in human tumor cell lines, SARs and effects on the cell cycle" Eur. J. Med. Chem. 45 (12): 5628-5634 (2010). http://dx.doi.org/10.1016/j.ejmech.2010.09.014

Queiroz MJ, Calhelha RC, Vale-Silva LA, Pinto E, São-José Nascimento M. “Novel 6-[(hetero)arylamino]thieno[3,2-b]pyridines: Synthesis and antitumoral activities” Eur. J. Med. Chem. 45 (12): 5732-5738 (2010). http://dx.doi.org/10.1016/j.ejmech.2010.09.030

Raposo MMM, García-Acosta B, Ábalos T, Martínez-Manez R, Ros-Lis JV, Soto J. "Synthesis and study of the use of heterocyclic thiosemicarbazones as signalling scaffolding for the recognition of anions" J. Org. Chem., 75 (9), 2922–2933. (2010). http://dx.doi.org/10.1021/jo100082k

Paiva MC, Simon F, Novais RM, Ferreira T, Proença MF, Xu W, Besenbacher F. “Controlled functionalization of carbon nanotubes by a solvent free multicomponent approach” ACS Nano 4 (12), 7379-7386. (2010). http://dx.doi.org/10.1021/nn1022523

Paiva MC, Novais RM, Araújo RF, Pederson KK, Proença MF, Silva CJR, Costa CM, Lanceros-Méndez S. “Organic functionalization of carbon nanofibres for composite applications” Polymer Composites, 31 (3): 369-376 (2010). http://dx.doi.org/10.1002/pc.20813

Salaheldin AM, Oliveira-Campos AMF, Parpot P, Rodrigues LM, Oliveira MM, Feixoto FP. “Synthesis of New Tacrine Analogues from 4-Amino-1H-pyrrole-3-carbonitrile”, Helv. Chim. Acta, 93 (2): 242-248 (2010). http://dx.doi.org/10.1002/hlca.200900190

Oliveira-Campos AMF, Ribeiro JMO, Rodrigues LM, Parpot P, Lopes PE. “3–{1–[(4–Methylphenyl)sulfonil]-1,4–dihydropyridin–4–yl}–1H– indole” Acta Crystallogr Sect E Struct Rep Online, 66 (Pt4): o915 (2010). http://dx.doi.org/10.1107/S1600536810010214

Oliveira-Campos AMF, Rodrigues LM, Esteves AP, Silva ME, Sivasubramanian A, Hrdina R, Soares GMB, Pinto TAD, Machalicky O. “Naphthotriazole derivatives: synthesis and fluorescence properties”, Dyes and Pigments, 87 (3): 188-193 (2010). http://dx.doi.org/10.1016/j.dyepig.2010.03.025

Pereira G, Castanheira EMS, Ferreira PMT, Queiroz M-JRP. “Synthesis and Photophysical Studies of New Fluorescent Indole Derivatives Obtained from β-Bromodehydroamino Acids – Interaction with Fluoride Anions” Eur. J. Org. Chem. 2010 (3): 464-475 (2010). http://dx.doi.org/10.1002/ejoc.200900737

Herbivo C, Comel A, Kirsch G, Fonseca AMC, Belsley M, Raposo MMM "Synthesis and characterization of novel, thermally stable 2-aryl-5-dicyanovinylthiophenes and 5-aryl-5'-dicyanovinyl-2,2'-bithiophenes as potentially promising non-linear optical materials", Dyes and Pigments 86 (3): 217-226 (2010). http://dx.doi.org/10.1016/j.dyepig.2010.01.006

Pina J, Seixas de Melo JS, Batista RM, Costa SP, Raposo MM. "Synthesis and characterization of the ground and excited states of tripodal-like oligothienyl-imidazoles", J. Phys. Chem. B., 114 (15): 4964-4972 (2010). http://dx.doi.org/10.1021/jp9104954

Fonseca AF, Belsley M, Gomes EM, Castro MCR, Raposo MMM. "Molybdenum Complexes Bearing (Bi)thienyl- or Arylthienyl-Substituted π-Conjugated Spacers: Synthesis, Electrochemical, Spectroscopic and Nonlinear Optical Properties ", Eur. J. Inorg. Chem. 2010 (19), 2998-3004 (2010). http://dx.doi.org/10.1002/ejic.201000218

Esteves CIC, Raposo MMM, Costa SPG. "Synthesis and evaluation of benzothiazolyl and benzimidazolyl asparagines as amino acid based selective fluorimetric chemosensors for Cu2+ ", Tetrahedron 66 (38): 7479-7486 (2010). http://dx.doi.org/10.1016/j.tet.2010.07.063

Monteiro LS, Kołomańska J, Suarez AC “Synthesis of Novel Nonproteinogenic Amino Acids: N-Ethyl-α,β-dehydroamino Acid Methyl Esters” Eur. J. Org. Chem., 2010 (35): 6731-6735 (2010). http://dx.doi.org/10.1002/ejoc.201001302

Ferreira PMT, Castanheira EMS, Monteiro LS, Pereira G, Vilaça H “A mild high yielding synthesis of oxazole-4-carboxylate derivatives”, Tetrahedron, 66 (45): 8672-8680 (2010). http://dx.doi.org/10.1016/j.tet.2010.09.014

Ferreira PM, Monteiro LS, Pereira G. “Synthesis and electrochemical behaviour of beta-halodehydroamino acid derivatives” Amino Acids 39 (2): 499-513 (2010). http://dx.doi.org/10.1007/s00726-009-0466-x

Soares AM, Costa SP, Gonçalves MS. “2-Oxo-2H-benzo[h]benzopyran as a new light sensitive protecting group for neurotransmitter amino acids”, Amino Acids, 39 (1): 121-133 (2010). http://dx.doi.org/10.1007/s00726-009-0383-z

Fonseca AS, Gonçalves MS, Costa SP. “Light-induced cleavage of model phenylalanine conjugates based on coumarins and quinolones”, Amino Acids, 39 (3): 699-712 (2010). http://dx.doi.org/10.1007/s00726-010-0492-8

Soares AMS, Costa SPG, Gonçalves MST. “Oxazole light triggered protecting groups: synthesis and photolysis of fused heteroaromatic conjugates”, Tetrahedron, 66 (41): 8189-8195 (2010). http://dx.doi.org/10.1016/j.tet.2010.08.020

Hungerford G, Ryderfors L, Fernandes MJG, Gonçalves MST, Costa SPG. “One- and two-photon time-resolved fluorescence study of neurotransmitter amino acid – 5,6-benzocoumarin conjugates”, J. Photochem. Photobiol. A: Chemistry, 215 (2-3): 214–222 (2010). http://dx.doi.org/10.1016/j.jphotochem.2010.08.020

Arsénio de Sá, M. Áurea A. Martins, Isabel M. Prata, Carlos F. G. C. Geraldes, P.M.T. Ferreira, João P. André “Gallium labeled NOTA-based conjugates for peptide receptor-mediated medical imaging” Bioorg. Med. Chem. Lett., 20, 7345–7348 (2010). http://dx.doi.org/10.1016/j.bmcl.2010.10.059

C. Gonçalves, M.F.M. Ferreira, A.C. Santos, M.I.M. Prata, C.F.G.C. Geraldes, J. A. Martins and F.M. Gama “Studies on the biodistribution of dextrin nanoparticles” Nanotechnology, 21, 295103 (2010). http://dx.doi.org/10.1088/0957-4484/21/29/295103

Arsénio de Sá, M. Isabel M. Prata, Carlos F. G. C. Geraldes, João P. André “Triaza-based amphiphilic chelators: synthetic route, in vitro characterization and in vivo studies of their Ga(III) and Al(III) chelates” J. Inorg. Biochem., 104, 1051-1062 (2010). http://dx.doi.org/10.1016/j.jinorgbio.2010.06.002

Monteiro LS, Andrade JJ, Suárez AC “Synthesis of New N-Ethyl Dehydroamino Acid Derivatives: N-Ethyl β,β-Dibromo, N-Ethyl β-Bromo β-Substituted, and N-Ethyl β,β-Disubstituted N-Protected Dehydroamino Acid Methyl Esters” Eur. J. Org. Chem., 2011 (33): 6764-6772 (2011). http://dx.doi.org/10.1002/ejoc.201100907

Ferreira PMT, Monteiro LS, Castanheira EMS, Pereira G, Lopes C, Vilaça H “Electrochemical reduction of dehydroamino acids: synthesis and photophysical properties of β,β-diarylalanines”, Tetrahedron, 67 (1): 193-200 (2011). http://dx.doi.org/10.1016/j.tet.2010.10.087

Naik S, Alves CMA, Coutinho PJG, Gonçalves MST. “N-(Di)icosyl-Substituted Benzo[a]phenoxazinium Chlorides: Synthesis and Evaluation as Near-Infrared Membrane Probes”, Eur. J. Org. Chem. 2011, (13): 2491-2497 (2011). http://dx.doi.org/10.1002/ejoc.201001579.

Alves CMA, Naik S, Coutinho PJG, Gonçalves MST. “Novel DNA fluorescence probes based on N-[5-(11-functionalised-undecylamino)-9H-benzo[a]phenoxazin-9-ylidene]propan-1-aminium chlorides: synthesis and photophysical studies”, Tetrahedron Letters 52 (1): 112–116 (2011). http://dx.doi.org/10.1016/j.tetlet.2010.10.165

Fernandes MJG, Costa SPG, Gonçalves MST. “Phototriggering of neuroactive amino acids from 5,6-benzocoumarinyl conjugates”, Tetrahedron 67 (13): 2422-2426 (2011). http://dx.doi.org/10.1016/j.tet.2011.01.090

Piloto AM, Soares AMS, Hungerford G, Costa SPG, Gonçalves MST. “Long-wavelength photolysis of amino acid 6-(methoxy-2-oxo-2H-naphtho[1,2-b]pyran-4-yl)methyl esters” Eur. J. Org. Chem. 2011 (28): 5447-5451 (2011). http://dx.doi.org/10.1002/ejoc.201100391

Queiroz M-J.R.P., Calhelha RC, Vale-Silva LA, Pinto E, Almeida GM, Vasconcelos MH. “Synthesis and Evaluation of Tumor Cell Growth Inhibition of Methyl 3-Amino-6-[(hetero)arylethynyl]thieno[3,2-b]pyridine-2-carboxylates. Structure-Activity Relationships, Effects on the Cell Cycle and Apoptosis” Eur. J. Med. Chem. 46, (1): 236-240 (2011). http://dx.doi.org/10.1016/j.ejmech.2010.11.009

Begouin A, Queiroz M.-J.R.P. “Tandem Palladium/Charcoal-Copper(I) Iodide (Pd/C-CuI) Catalyzed Sonogashira Coupling and Intramolecular Cyclization from 2-Bromonicotinic Acid (=2-Bromopyridine-3-carboxylic Acid) and Ethynylarenes to 4-Azaphthalides (=Furo[3,4-b]pyridin-5(7H)-ones) and 5-Azaisocoumarins (=5H-Pyrano[4,3-b]pyridin-5-ones)” Helvetica Chimica Acta, 94, (10): 1792-1801 (2011). http://dx.doi.org/10.1002/hlca.201100060

Hermenegildo BF, Pereira G, Abreu AS, Castanheira EMS, Ferreira PMT, Queiroz M-J.R.P. “Phenanthrenyl-indole as a fluorescent probe for peptides and lipid membranes” J. Photochem. Photobiol. A: Chemistry, 221 (1): 47-57. http://dx.doi.org/10.1016/j.jphotochem.2011.04.022

Dias AM, Vila-Chã AS, Costa AL, Cunha DP, Senhorães N, Proença MF. “Versatile Synthesis of 5-Aminoimidazole-4-carboxylic Acid Derivatives” Synlett 2011 (18): 2675-2680 (2011). http://dx.doi.org/10.1055/s-0031-1289528

Raposo MMM, Fonseca AMC, Castro MCR, Belsley M, Cardoso MFS, Carvalho LM, Coelho PJ. “Synthesis and characterization of novel diazenes bearing pyrrole, thiophene and thiazole heterocycles as efficient

photochromic and nonlinear optical (NLO) materials", Dyes and Pigments, 91, (1): 62-73 (2011). http://dx.doi.org/10.1016/j.dyepig.2011.02.012

Raposo MMM, Castro MCR, Fonseca AMC, Schellenberg P, Belsley M. "Design, synthesis, and characterization of the electrochemical, nonlinear optical properties, and theoretical studies of novel thienylpyrrole azo dyes bearing benzothiazole acceptor groups", Tetrahedron 67 (29): 5189-5198 (2011). http://dx.doi.org/10.1016/j.tet.2011.05.053

Raposo MMM, Castro MCR, Belsley M, Fonseca AMC. "Push–pull bithiophene azo-chromophores bearing thiazole and benzothiazole acceptor moieties: Synthesis and evaluation of their redox and nonlinear optical properties", Dyes and Pigments, 91, (3), 454-465 (2011). http://dx.doi.org/10.1016/j.dyepig.2011.05.007

Esteves CI, Raposo MM, Costa SP. "Novel highly emissive non-proteinogenic amino acids: synthesis of 1,3,4-thiadiazolyl asparagines and evaluation as fluorimetric chemosensors for biologically relevant transition metal cations", Amino Acids 40, (4): 1065-1075 (2011). http://dx.doi.org/10.1007/s00726-010-0730-0

Batista RMF, Oliveira E, Costa SPG, Lodeiro C, Raposo MMM " Imidazo-benzo-15-crown-5 ethers bearing arylthienyl and bithienyl moieties as novel fluorescent chemosensors for Pd2+ and Cu2+", Tetrahedron 67, (37): 7106-7113 (2011). http://dx.doi.org/10.1016/j.tet.2011.06.106

Oliveira E, Genovese D, Juris R, Zaccheroni N, Capelo JL, Raposo MM, Costa SP, Prodi L, Lodeiro C. "Bioinspired systems for metal-ion sensing: new emissive peptide probes based on benzo[d]oxazole derivatives and their gold and silica nanoparticles", Inorg. Chem., 50, (18): 8834-49 (2011). http://dx.doi.org/10.1021/ic200792t

Batista RMF, Oliveira E, Costa SPG, Lodeiro C, Raposo MMM "(Oligo)thienyl-imidazo-benzocrown ether derivatives: Synthesis, photophysical studies and evaluation of their chemosensory properties", Talanta, 85 (5), 2470-2478 (2011). http://dx.doi.org/10.1016/j.talanta.2011.07.107

Alves MJ, Costa FT, Duarte VCM, Fortes AG, Martins JA, Micaelo NM. "Advances in the Synthesis of Homochiral (–)-1-Azafagomine and (+)-5-epi-1-Azafagomine. 1-N-Phenyl Carboxamide Derivatives of both Enantiomers of 1-Azafagomine: Leads for the Synthesis of Active α-Glycosidase Inhibitors" J Org. Chem. 76, (23) 9584-9592 (2011). http://dx.doi.org/10.1021/jo201486q

Senhorães N, Dias AM, Conde LM, Proença MF. "One-Pot Regioselective Synthesis of 2,6,9-Trisubstituted Adenines" Synlett 2011 (2): 181-186 (2011). http://dx.doi.org/10.1055/s-0030-1259289

Zaki MEA, Proença MF. "Synthesis of 6-cyano and 6-unsubstituted 2-aryl-8-oxopurine from a common 2-oxoimidazole precursor" Tetrahedron 67, (4): 755-762 (2011). http://dx.doi.org/10.1016/j.tet.2010.11.064

Proença F, Costa M. "A one-pot synthesis of substituted pyrido[2,3-b]indolizines" Tetrahedron, 67, (6), 1071-1075 (2011). http://dx.doi.org/10.1016/j.tet.2010.12.047

Costa M, Proença F. " 2-Aryl-1,9-dihydrochromeno[3,2-d]imidazoles: a facile synthesis from salicylaldehydes and arylideneaminoacetonitrile" Tetrahedron 67, (10), 1799-1804 (2011). http://dx.doi.org/10.1016/j.tet.2011.01.035

Costa M, Areias F, Castro M, Brea J, Loza MI, Proença F. "Synthesis of novel chromene scaffolds for adenosine receptors" Org. Biomol Chem. 9, 4242-4249 (2011). http://dx.doi.org/10.1039/C1OB05305A

Costa M, Proença MF. "Selective synthesis of some imidazopyridine-fused chromones" Tetrahedron, 67 (45): 8622-8627 (2011). http://dx.doi.org/10.1016/j.tet.2011.09.054

Calhelha RC, Ferreira ICFR, Peixoto D, Abreu RMV, Vale-Silva LA, Pinto E, Lima RT, Alvelos MI, Vasconcelos MH, Queiroz M-JR P. "Aminodi(hetero)arylamines in the Thieno[3,2-b]pyridine Series: Synthesis, Effects in Human Tumor Cells Growth, Cell Cycle Analysis, Apoptosis and Evaluation of Toxicity Using Non-Tumor Cells" Molecules, 17 (4): 3834-3843 (2012). http://dx.doi.org/10.3390/molecules17043834

Queiroz M-JRP, Dias S, Peixoto D, Rodrigues ARO, Oliveira ADS, Coutinho PJG, Vale-Silva LA, Pinto E, Castanheira EMS "New potential antitumoral di(hetero)arylether derivatives in the thieno[3,2-b]pyridine series: synthesis and fluorescence studies in solution and in nanoliposomes" J. Photochem. Photobiol. A - Chem., 238, 71-80 (2012). http://dx.doi.org/10.1016/j.jphotochem.2012.04.007

Peixoto D, Begouin A, Queiroz M-JRP "Synthesis of 2-(hetero)arylthieno[2,3-b] or [3,2-b]pyridines from 2,3-

dihalopyridines, (hetero)arylalkynes and Na2S. Further functionalizations" Tetrahedron, 68, 7082-7094 (2012). http://dx.doi.org/10.1016/j.tet.2012.06.057

Salgueiro DAL, Duarte VCM, Sousa CEA, Alves MJ, Gil Fortes A. "Diastereo-selectivity in Diels–Alder Cycloadditions of Erythrose Benzylidene-acetal 1,3-Butadienes with Maleimides", Synlett, 23: 1765-1768 (2012). http://dx.doi.org/10.1055/s-0031-1289785

Genin E, Hugues V, Clermont G, Herbivo C, Castro MCR, Comel A, Raposo MMM, Blanchard-Desce M. "Fluorescence and two-photon absorption of push-pull aryl(bi)thiophenes: structure-property relationships", Photochem. Photobiol. Sci., 11 (11): 1756-1766 (2012). http://dx.doi.org/10.1039/c2pp25258a

Correia C, Carvalho MA, Rocha A, Proença MF. "General Synthetic Approach to 2-Phenolic Adenine Derivatives", Synlett 2012, 1923-1926 (2012) http://dx.doi.org/10.1055/s-0031-1290694

Salgueiro DAL, Sousa CEA, Gil Fortes A, Alves MJ. "Diels-Alder Cycloaddition in the Synthesis of 1-Azafagomine, Analogues, and Derivatives as Glycosidase Inhibitors", Mini Reviews in Med. Chem., 12: 1465-1476 (2012). http://dx.doi.org/10.2174/138955712803832663

Costa M, Areias F, Castro M, Brea J, Mestres J, Proença F, Loza M. "A new chromene scaffold for adenosine A2A receptors. Synthesis, pharmacology, and structure-activity relationships" Eur. J. Med. Chem., 54: 303-310 (2012). http://dx.doi.org/10.1016/j.ejmech.2012.05.009

Dias TA, Proença MF. "An ecofriendly approach to the synthesis of the 3-phenylsulfonyl-2H-chromene scaffold" Tetrahedron Letters, 53 (39): 5235-5237 (2012). http://dx.doi.org/10.1016/j.tetlet.2012.07.069

Sivasubramanian A, Narasimha KKG, Rathnasamy R, Oliveira Campos AM. "A new antifeedant clerodane diterpenoid from Tinospora cordifolia", Natural Product Research, 2012: 1–6, (2012). http://dx.doi.org/10.1080/14786419.2012.722088

Pedras B, Batista RMF, Tormo L, Costa SPG, Raposo MMM, Orellana G, Capelo JL, Lodeiro C. "New Ru(II) Thienyl-imidazo-phenanthroline polypyridyl complexes: synthesis, characterization, photophysical studies and interaction with DNA", Inorg. Chim. Acta, 381, 95-103 (2012). http://dx.doi.org/10.1016/j.ica.2011.07.020

Santos-Figueroa LE, Moragues ME, Raposo MMM, Batista RMF, Ferreira RCM, Costa SPG, Sancenón F, Martínez-Máñez R, Ros-Lis JV, Soto J. "Synthesis and evaluation of fluorimetric and colorimetric chemosensors for anions based on (oligo)thienyl-thiosemicarbazones" Tetrahedron, 68 (35): 7179-7186 (2012). http://dx.doi.org/10.1016/j.tet.2012.06.021

Batista RMF, Ferreira RCM, Raposo MMM, Costa SPG. "Novel optical chemosensors for anion and cations based on an amino acid core functionalised with benzimidazoles", Tetrahedron, 2012, 68 (36): 7322-7330 (2012). http://dx.doi.org/10.1016/j.tet.2012.06.087

Santos-Figueroa LE, Moragues ME, Raposo MMM, Batista RMF, Ferreira RCM, Costa SPG, Sancenón F, Martínez-Máñez R, Ros-Lis JV, Soto J. "Synthesis and evaluation of thiosemicarbazones functionalized with furyl moieties as new chemosensors for anion recognition", Org Biomol Chem; 10 (36), 7418-7428 (2012). http://dx.doi.org/10.1039/c2ob26200b

Pinto TAD, Hrdina R, Kirsch G, Oliveira-Campos AMF, Rodrigues LM, Esteves AP. "Synthesis of esters derived from 2,3,4-tri-O-benzyl-alpha-D-methylglucoside", ARKIVOC, 2012, Part 6, 185-193 (2012).

Gonçalves MST, Oliveira-Campos AMF, Rodrigues LM, Proença MFRP. "Synthesis of 4-amino-3,5-dicyano-arylpyrazoles. Part 2: isolation and characterization of byproducts", Synth. Commun., 42 (11): 1695-1703 (2012). http://dx.doi.org/10.1080/00397911.2010.543304

Francisco CS, Rodrigues LR, Cerqueira NMFSA, Oliveira-Campos AMF, Rodrigues LM. "Synthesis of novel benzofurocoumarin analogues and their anti-proliferative effecton human cancer cell lines", Eur. J. Med. Chem., 47: 370-376 (2012). http://dx.doi.org/10.1016/j.ejmech.2011.11.005

Castro MCR, Schellenberg P, Belsley M, Fonseca AMC, Fernandes SSM, Raposo MMM. "Design, synthesis and evaluation of redox, second order nonlinear optical properties and theoretical DFT studies of novel bithiophene azo dyes functionalized with dithiazole acceptor groups", Dyes Pigments 95 (2), 392-399 (2012). http://dx.doi.org/10.1016/j.dyepig.2012.05.014

Coelho P, Castro MCR, Fonseca AMC, Fernandes SSM, Raposo MMM. "Enhancement of the photochromic switching speed of bithiophene azo dyes", Tetrahedron

Lett., 53 (34), 4502-4506 (2012). http://dx.doi.org/10.1016/j.tetlet.2012.05.166

Castro MCR, Belsley M, Fonseca AMC, Raposo MMM. "Synthesis and characterization of novel second-order NLO-chromophores bearing pyrrole as an electron donor group", Tetrahedron, 68 (39), 8147-8155 (2012). http://dx.doi.org/10.1016/j.tet.2012.07.082

Kuźniarska-Biernacka I, Rodrigues O, Carvalho MA, Neves IC, Fonseca AM. "Encapsulation of manganese(III) complex in NaY nanoporosity for heterogeneous catalysis", Appl. Organometal. Chem., 26, 44–49 (2012). http://dx.doi.org/10.1002/aoc.1865

Zaki MEA, Bettencourt AP, Fernandes FM, Proença MF. "Synthesis and Electrochemical Evaluation of Imidazo[4,5-d]pyrrolo[3,2-f][1,3]diazepine Scaffolds", Tetrahedron 68 (24): 4628-4634 (2012). http://dx.doi.org/10.1016/j.tet.2012.04.030

Piloto AM, Soares AMS, Costa SPG, Gonçalves MST. "Photorelease of amino acids from novel thioxobenzo[f]benzopyran ester conjugates", Amino Acids, 42 (6): 2275–2282 (2012). http://dx.doi.org/10.1007/s00726-011-0969-0

Soares AMS, Piloto AM, Hungerford G, Costa SPG, Gonçalves MST. "Photolytic release of butyric acid from oxygen and nitrogen based heteroaromatic cages", Eur. J. Org. Chem., 2012: 922–930 (2012). http://dx.doi.org/10.1002/ejoc.201101392

Fonseca ASC, Gonçalves MST, Costa SPG. "A photoactivable amino acid based on a novel functional coumarin-6-yl-alanine, Amino Acids, 43 (6): 2329–2338. (2012). http://dx.doi.org/10.1007/s00726-012-1310-2

Fonseca ASC, Gonçalves MST, Costa SPG. "Phenacyl ester derivatives bearing heterocycles as models for photocleavable linkers: synthesis and photolysis studies", Tetrahedron, 68 (38): 8024-8032 (2012). http://dx.doi.org/10.1016/j.tet.2012.06.100

Firmino ADG, Gonçalves MST. "Bifunctionalised long-wavelength fluorescent probes for biological applications", Tetrahedron Lett., 53 (37): 4946–4950 (2012). http://dx.doi.org/10.1016/j.tetlet.2012.07.004

Fonseca ASC, Soares AMS, Gonçalves MST, Costa SPG. "Thionatedcoumarins and quinolones in the light triggered release of a model amino acid: synthesis and photolysis studies", Tetrahedron, 68 (38): 7892-7900 (2012). http://dx.doi.org/10.1016/j.tet.2012.07.021

Monteiro LS, Suárez AC. "High yielding synthesis of N-ethyl dehydroamino acids" Amino Acids, 43 (4): 1643-1652 (2012) http://dx.doi.org/10.1007/s00726-012-1240-z

Ferreira MF, Mousavi B, Ferreira PM, Martins C, Helm L, Martins JA, Geraldes CFGC. "Gold nanoparticles functionalised with stable, fast exchanging Gd3+ chelates as high relaxivity Contrast Agents for MRI", Dalton Trans., 41: 5472-5475 (2012). http://dx.doi.org/10.1039/C2DT30388D

Pereira G, Ferreira MF, Castanheira EMS, Martins JA, Ferreira PMT "Synthesis of new 2,6-bis-(oxazolyl)pyridine ligands for luminescent Ln(III) complexes" Eur. J. Org. Chem. 2012 (21): 3950-3910 (2012). http://dx.doi.org/10.1002/ejoc.201200177

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Scientific Papers

Branco PC, Castilho PC, Rosa MF, Ferreira J. "Characterization of Annona cherimola Mill. Seed Oil from Madeira Island: a Possible Biodiesel Feedstock" J. Am. Oil Chem. Soc. 87 (4): 429-436 (2010). http://dx.doi.org/10.1007/s11746-009-1513-1

Jardim MG, Rissanen K, Rodrigues J. "Preparation and Characterization of Novel Poly(alkyliden imine) Nitrile Ruthenium Metallodendrimers" Eur. J. Inorg. Chem., 2010 (11): 1729-1735 (2010). http://dx.doi.org/10.1002/ejic.200901187

Santos JL, Pandita D, Rodrigues J, Pêgo AP, Granja PL, Balian G, Tomás H. "Receptor-mediated gene delivery using PAMAM dendrimers conjugated with peptides recognized by mesenchymal stem cells" Mol. Pharmaceutics, 7 (3): 763-774 (2010). http://dx.doi.org/10.1021/mp9002877

Santos JL, Oliveira H, Pandita D, Rodrigues J, Pêgo AP, Granja PL, Tomás H. "Functionalization of Poly(amidoamine) Dendrimers with hydrophobic chains for improved gene delivery in mesenchymal stem cells" J.

Control Release, 144 (1): 55-64 (2010). http://dx.doi.org/10.1016/j.jconrel.2010.01.034

Bonniard L, Kahlal S, Diallo AK, Ornelas C, Roisnel T, Manca G, Rodrigues J, Ruiz J, Astruc D, Saillard J-Y. "How Do Nitriles Compare with Isoelectronic Alkynyl Groups in the Electronic Communication between Iron Centers Bridged by Phenylenebis- and -tris(nitrile) Ligands? An Electronic and Crystal-Structure Study" Inorg. Chem., 50 (1): 114-124 (2011). http://dx.doi.org/10.1021/ic101415c

Pandita D, Santos JL, Rodrigues J, Pêgo AP, Granja PL, Tomás H "Gene Delivery into Mesenchymal Stem Cells: A Biomimetic Approach Using RGD Nanoclusters Based on Poly(amidoamine) Dendrimers" Biomacromolecules, 12 (2): 472-481 (2011). http://dx.doi.org/10.1021/bm1012647

Rodrigues J, Jardim MG, Figueira J, Gouveia M, Tomás H, Rissanen K. "Poly(alkylidenamines) dendrimers as scaffolds for the preparation of low-generation ruthenium based metallodendrimers" New. J. Chem. 35, 1938–1943 (2011). http://dx.doi.org/10.1039/C1NJ20364A

Gonçalves M, Castro R, Rodrigues J, Tomás H. "The Effect of PAMAM Dendrimers on Mesenchymal Stem Cell Viability and Differentiation" Curr. Med. Chem., 19: 4969-4975 (2012). http://dx.doi.org/10.2174/092986731120902496 9

Nouri A, Castro R, Kairys V, Santos JL, Rodrigues J, Li Y, Tomás H. "Insight into the role of N, N-dimethylaminoethyl methacrylate (DMAEMA) conjugation onto poly (ethylenimine): cell viability and gene transfection studies", J. Mater Sci: Mater. M., 23 (12): 2967-2980 (2012). http://dx.doi.org/10.1007/s10856-012-4753-9

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Scientific Papers

Nacira Darghal, Arlette Garnier-Suillerot, Nadia Bouchemal, Gabriel Grasc, Carlos F.G. C. Geraldes, Milena Salerno "Accumulation of Eu3+ Chelates in Cells Expressing or not P-Glycoprotein: Implications for Blood Brain Barrier Crossing" J. Inorg. Biochem., 104, 47-54 (2010). http://dx.doi.org/10.1016/j.jinorgbio.2009.09.026

Carvalho JFS, Cruz Silva MM, Moreira JN, Simões S, Melo MLS. "Selective Cytotoxicity of Oxysterols through Structural Modulation on Rings A and B. Synthesis, in vitro evaluation and SAR" J. Med. Chem. 54, (18): 6375-6393 (2011). http://dx.doi.org/10.1021/jm200803d

Dąbrowski JM, Krzykawska M, Arnaut LG, Pereira MM, Monteiro CJ, Simões S, Urbańska K, Stochel G. "Tissue Uptake Study and Photodynamic Therapy of Melanoma-Bearing Mice with a Nontoxic, Effective Chlorin" Chem. Med. Chem. 6, (9): 1715-1726 (2011). http://dx.doi.org/10.1002/cmdc.201100186

Moreira VM, Salvador JA, Beja AM, Paixão JA. "The Reaction of Azoles with 17-Chloro-16-formylandrosta-5,16-dien-3β-yl-acetate: Synthesis and Structural Elucidation of Novel 16-Azolylmethylene-17-oxoandrostanes" Steroids 76, (6): 582–587 (2011). http://dx.doi.org/10.1016/j.steroids.2011.02.009

Pereira NAM, Fonseca SM, Serra AC, Pinho e Melo TMVD, Burrows HD. "Cycloaddition of meso- Tetra- and 5,15-Di-Arylporphyrins: Synthesis and Photophysical Characterization of Stable Chlorins and Bacteriochlorins" Eur. J. Org. Chem. 2011, (20-21): 3970-3979 (2011). http://dx.doi.org/10.1002/ejoc.201100465

Soares MIL, Gomes CSB, Pinho e Melo TMVD. "Nitrogen-bridged heterocycles via cycloaddition of non-classical heterocyclic-fused-[c]thiazoles" Tetrahedron 67, (43): 8392-8403 (2011). http://dx.doi.org/10.1016/j.tet.2011.08.001

Cardoso AL, Nunes RMD, Arnaut LG, Pinho e Melo TMVD "Synthesis of Pyrroles in Supercritical Carbon Dioxide: Formal [3+2] Cycloaddition of 2-Benzoyl-Aziridines and Allenoates" Synthesis 2011, (21): 3516-3522 (2011). http://dx.doi.org/10.1055/s-0030-1260209

Lopes SMM, Palacios F, Lemos A, Pinho e Melo TMVD. "Diels–Alder reactions of 3-(1H-tetrazol-5-yl)-nitrosoalkenes: synthesis of functionalized 5-(substituted)-1H-tetrazoles" Tetrahedron 67, (46): 8902-8909 (2011). http://dx.doi.org/10.1016/j.tet.2011.09.051

Nunes CM, Reva I, Pinho e Melo TM, Fausto R, Šolomek T, Bally T. "The pyrolysis of isoxazole revisited: a new primary product and the pivotal role of the vinylnitrene. A low-temperature matrix isolation and computational study" J. Am. Chem. Soc. 133, (46): 18911-18923 (2011). http://dx.doi.org/10.1021/ja207717k

Serra AC, d'A. Rocha Gonsalves AM. "Mild oxygen activation with isobutyraldehyde promoted by simple salts"

Tetrahedron Lett. 52, (27): 3489–3491 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.04.120

Ribeiro SM, Serra AC, d'A. Rocha Gonsalves AM. "Silica grafted polyethylenimine as heterogeneous catalyst for condensation reactions" Applied Catalysis A: General 399, (1-2): 126–133 (2011). http://dx.doi.org/10.1016/j.apcata.2011.03.054

Mendes S, Camacho F, Silva T, Calado CR, Serra AC, Gonsalves AM, Roxo-Rosa M. "A nonionic Porphyrin as a Noninterfering DNA Antibacterial Agent" Photochem Photobiol. 87, (6): 1395-1404 (2011). http://dx.doi.org/10.1111/j.1751-1097.2011.00984.x

Carvalho JFS, Cruz Silva MM, Sa e Melo ML. "Efficient trans-diaxial hydroxylation of Δ5-steroids" Tetrahedron 66, (13): 2455-2462 (2010). http://dx.doi.org/10.1016/j.tet.2010.01.089

Serra ME, Murtinho D, Goth A, Rocha Gonsalves AM, Abreu PE, Pais AA. "Ultrasound-mediated synthesis of camphoric acid-based chiral salens for the enantioselective trimethylsilylcyanation of aldehydes" Chirality 22, (4): 425-31 (2010). http://dx.doi.org/10.1002/chir.20758

Serra MES, Murtinho D, Goth A. "Enantioselective trimethylsilylcyanation of benzaldehyde using pyrrolidine-based chiral salen ligands" Arkivoc 2010 (v): 64-69 (2010). http://dx.doi.org/10.3998/ark.5550190.0011.507

Murtinho D, Serra MES, Rocha Gonsalves AMd'a. "Enantioselective ethylation of aldehydes with 1,3-N-donor ligands derived from (+)-camphoric acid" Tetrahedron: Asymmetry 21 (1): 62-68 (2010). http://dx.doi.org/10.1016/j.tetasy.2009.12.012

Pereira N, Serra AC, Pineiro M, Rocha Gonsalves AMd'a, Abrantes M, Laranjo M, Botelho F. "Synthetic porphyrins bearing β-propionate chains as photosensititizers for photodynamic therapy" Journal of Porphyrins and Phthalocyanines, 14 (5): 438-445 (2010). http://dx.doi.org/10.1142/S1088424610002227

Serra AC, Rocha Gonsalves AMd'a. "Controlled porphyrinogen oxidation for the selective synthesis of meso-tetraarylchlorins" Tetrahedron Letters 51 (32): 4192-94 (2010). http://dx.doi.org/10.1016/j.tetlet.2010.06.010

Ribeiro SM, Serra AC, Rocha Gonsalves AMd'a. "Covalently immobilized porphyrins on silica modified structures as photooxidation catalysts" Journal of Molecular Catalysis A: Chemical, 326 (1-2): 121-127 (2010). http://dx.doi.org/10.1016/j.molcata.2010.05.001

Serra A, Pineiro M, Santos CI, Gonsalves AM, Abrantes M, Laranjo M, Botelho MF. "In vitro photodynamic activity of 5,15-bis(3-hydroxyphenyl)porphyrin and its halogenated derivatives against cancer cells" Photochem Photobiol., 86 (1): 206-12 (2010). http://dx.doi.org/10.1111/j.1751-1097.2009.00622.x

Pineiro M, Ribeiro SM, Serra AC. "The influence of the support on the singlet oxygen quantum yields of porphyrin supported photosensitizers" Arkivoc 2010 (V): 51-63 (2010).

Lopes SMM, Santos BS, Palacios F, Pinho e Melo TMVD "Microwave-assisted reactions of allenic esters: [3+2] anellations and allenoate-Claisen rearrangement" Arkivoc 2010 (V): 70-81 (2010).

Nunes CM, Silva MR, Beja AM, Fausto R, Pinho e Melo TMVD "Cycloaddition of trifluoromethyl azafulvenium methides: synthesis of new trifluoromethylpyrrole-annulated derivatives" Tetrahedron Letters 51 (2): 411-414 (2010). http://dx.doi.org/10.1016/j.tetlet.2009.11.033

Lopes SMM, Laranjo M, Serra AC, Abrantes AM, Rocha Gonsalves AMd'a, Botelho MF, Beja AM, Silva MR, Pinho e Melo TMVD "Synthesis and Bilogical Evaluation of New Naphthoquinone-containing Pyrrolo-Thiazoles as Anticancer Agents" J. Heterocyclic Chem., 47 (4): 960-966 (2010). http://dx.doi.org/10.1002/jhet.396

Santos BS, Cardoso AL, Beja AM, Silva MR, Paixao JA, Palacios F, Pinho e Melo TMVD. "Diastereoselective Aza-Baylis–Hillman Reactions: Synthesis of Chiral α-Allenylamines and 2-Azetines from Allenic Esters" Eur. J. Org. Chem., 2010 (17): 3249-3256 (2010). http://dx.doi.org/10.1002/ejoc.200901415

Lopes SMM, Nunes CM, Pinho e Melo TMVD. "4-Isoxazolines and pyrroles from allenoates" Tetrahedron 66 (32): 6078-6084 (2010). http://dx.doi.org/10.1016/j.tet.2010.06.010

Cardoso AL, Beja AM, Silva MR,, de los Santos JM, Palacios F, Abreu PE, Pais AACC, Pinho e Melo TMVD "Stereoselective formation of tertiary and quaternary carbon centers via inverse conjugate addition of carbonucleophiles to allenic esters" Tetrahedron 66 (39): 7720-7725 (2010). http://dx.doi.org/10.1016/j.tet.2010.08.002

Soares MI, Brito AF, Laranjo M, Abrantes AM, Botelho MF, Paixão JA, Beja AM, Silva MR, Pinho E Melo TM. "Chiral 6-hydroxymethyl-1H,3H-pyrrolo[1,2-c]thiazoles: novel antitumor DNA monoalkylating agents" Eur J Med Chem., 45 (10): 4676-81 (2010). http://dx.doi.org/10.1016/j.ejmech.2010.07.029

Pereira NAM, Serra AC, Pinho E Melo TM. "Novel Approach to Chlorins and Bacteriochlorins: [8π+2π] Cycloaddition of Diazafulvenium Methides with Porphyrins" Eur. J. Org. Chem., 2010 (34): 6539-6543 (2010). http://dx.doi.org/10.1002/ejoc.201001157

Laia FMR, Cardoso AL, Beja AM, Silva MR, Pinho E Melo TMVD. "Reactivity of allenoates towards aziridines: synthesis of functionalized methylenepyrrolidines and pyrroles" Tetrahedron 66, (46): 8815-8822 (2010). http://dx.doi.org/10.1016/j.tet.2010.09.081

Lopes SMM, Lemos A, Pinho e Melo TMVD. "A hetero-Diels–Alder approach to functionalized 1H-tetrazoles: synthesis of tetrazolyl-1,2-oxazines, -oximes and 5-(1-aminoalkyl)-1H-tetrazoles" Tetrahedron Letters 51 (51): 6756-6759 (2010). http://dx.doi.org/10.1016/j.tetlet.2010.10.095

Gonsalves AR, Pineiro M, Martins JM, Barata PA, Menezes JC. "Identification of Alprazolam and its degradation products using LC-MS-MS" Arkivoc 2010 (V): 128-141 (2010).

Nascimento BFO, d'A. Rocha Gonsalves AM, Pineiro M "MnO2 instead of quinones as selective oxidant of tetrapyrrolic macrocycles" Inorg Chem Comm., 13, (3): 395-398 (2010). http://dx.doi.org/10.1016/j.inoche.2009.12.032

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Book Chapters

Prejmerean C, Buruiana T, Nunes T, Moldovan M, Colceriu L "Biocomposites Based on New Monomer Systems Reinforced with Micro / Nanoparticles and Glass Fibers" in Metal, Ceramic and Polymeric Composites for Various Uses, pages 239-264, Edited by John Cuppoletti, July 2011, ISBN 978-953-307-353-8.

Pereira SA, Marques MM, Caixas U, Monteiro EC, Beland FA, Antunes AMM "Understanding the molecular basis for the hazards associated with nevirapine treatment" in Advances in Medicine and Biology, vol. 44 (Berhardt, L.V., ed.), Nova Science Publishers Inc., Hauppauge NY, 2012, ISBN 978-1-62100-961-0.

Pereira SA, Wanke R, Marques MM, Monteiro EC, Antunes AMM. "Insights into the Role of Bioactivation Mechanisms in the Toxic Events Elicited by Non-nucleoside Reverse Transcriptase Inhibitors" in Advances in Molecular Toxicology, vol. 6 (Fishbein, J.C., ed.), Elsevier B.V, pp 1-40 (2012), ISBN: 9780444593894.

Scientific Papers

Antunes MA, Namorado S, Azevedo CG, Lemos MA, Duarte MT, Ascenso JR, Martins AM "Pentabenzylcyclopentadienyl molybdenum and tungsten hydrides: Syntheses, structures and electrochemistry of [MHCpBz(CO)(2)(L)] (L = CO, PMe3, PPh3)" Journal of Organometallic Chemistry, 695, 1328-1336 (2010). http://dx.doi.org/10.1016/j.jorganchem.2010.02.012

Matos I, Fernandes A, Catalão R, Rego AMB, Ascenso JR, Fonseca IF, Lemos F, Marques MM "Heterogeneization of alpha diimines nickel catalysts for the polymerization of ethylene and methylmethacrylate" e-Polymers, 147, 1-18 (2010). ISSN 1618-7229

Pereira SG, Fulgêncio R, Nunes TG, Toledano M, Osorio R, Carvalho RM, "Effect of curing protocol on the polymerization of dual-cured resin cements", Dental Materials, 26, 710-718 (2010). http://dx.doi.org/10.1016/j.dental.2010.03.016

Nunes TG, Diogo HP, Pinto SS, Moura Ramos JJ "Molecular Dynamics of Amorphous Gentiobiose Studied by Solid-State NMR", J. Phys. Chem. B, 114, 15976-84, (2010). http://dx.doi.org/10.1021/jp106371w

Saraiva MS, Nunes CD, Nunes TG, Calhorda MJ "The effect of immobilization on the catalytic activity of molybdenum eta(3)-allyldicarbonyl complexes with nitrogen donor ligands bearing N-H groups" J. Molecular Catalysis A: Chemical, 321, 92-100, (2010). http://dx.doi.org/10.1016/j.molcata.2010.02.008

Vicente AI, Pereira SG, Nunes TG, Ribeiro MR "1H-NMR Study of Maleic Anhydride Modified Ethylene-Diene

Copolymers" J Polym Res, 18: 527-532 (2011). http://dx.doi.org/10.1007/s10965-010-9445-x

Fernandes CI, Silva NU, Vaz PD, Nunes TG, Nunes CD "Bio-inspired Mo(II) complexes as active catalysts in homogeneous and heterogeneous olefin epoxidation" Applied Catalysis A: General 384,(1-2): 84-93 (2010). http://dx.doi.org/10.1016/j.apcata.2010.06.011

Sousa SCA, Fernandes AC "Efficient and Highly Chemoselective Direct Reductive Amination of Aldehydes using the System Silane/Oxorhenium Complexes" Adv. Synth. Catal. 352, 2218-2226 (2010). http://dx.doi.org/10.1002/adsc.201000246

Cabrita I, Sousa SCA, Fernandes AC "Reduction of Sulfoxides Catalyzed by Oxo-complexes" Tetrahedron Letters 51, (47): 6132-6135 (2010). http://dx.doi.org/10.1016/j.tetlet.2010.09.071

Anisimova TB, Bokach NA, Luzyanin KV, Haukka M, Kukushkin VY "Push-pull nitrile ligands exhibit specific hydration patterns" Dalton Trans. 39, 10790–10798 (2010). http://dx.doi.org/10.1039/C0DT00711K

Silva TFS, Luzyanin KV, Kirillova MV, da Silva MFG, Martins LMDRS, Pombeiro AJL "Novel Scorpionate and Pyrazole Dioxovanadium Complexes, Catalysts for Carboxylation and Peroxidative Oxidation of Alkanes" Adv. Synth. Catal, 352 (1), 171–187. http://dx.doi.org/10.1002/adsc.200900660

da Silva JLF, Galvao AC, Ferreira AP, Galvão AM, Dias AR, Gomes PT, Salema MS "Effect of ancillary ligands in the hapticity of the pyrrolyl ligand in [Ti(pyrrolyl)(NMe2)(x)Cl3-x] (x=0, 1, 2, 3) complexes" Journal of Organometallic Chemistry, 695, 1533-40 (2010). http://dx.doi.org/10.1016/j.jorganchem.2010.03.007

Gomes CSB, Suresh D, Gomes PT, Veiros LF, Duarte MT, Nunes TG, Oliveira MC "Sodium complexes containing 2-iminopyrrolyl ligands: the influence of steric hindrance in the formation of coordination polymers" Dalton Transactions, 39 (3), 736-748 (2010). http://dx.doi.org/10.1039/b905948b

Lourenço AB, Ascenso JR, Sá-Correia I "Metabolic insights into the yeast response to propionic acid based on high resolution 1H NMR spectroscopy" Metabolomics 7, 457-468 (2011). http://dx.doi.org/10.1007/s11306-010-0264-1

Antunes AM, Godinho AL, Martins IL, Oliveira MC, Gomes RA, Coelho AV, Beland FA, Marques MM. "Protein adducts as prospective biomarkers of nevirapine toxicity" Chem Res Toxicol, 23 (11): 1714–1725 (2010). http://dx.doi.org/10.1021/tx100186t

Antunes AM, Godinho AL, Martins IL, Justino GC, Beland FA, Marques MM "Amino acid adduct formation by the nevirapine metabolite, 12-hydroxynevirapine – a possible factor in nevirapine toxicity" Chem. Res. Toxicol., 23 (5): 888–899 (2010). http://dx.doi.org/10.1021/tx900443z

Lidong L, Gomes CSB, Lopes PS, Gomes PT, Diogo HP, Ascenso JR. "Polymerization of styrene with tetradentate chelated a-diimine nickel(II) complexes/MAO catalyst systems: Catalytic behavior and microstructure of polystyrene" European Polymer Journal 47 (8): 1636–1645 (2011). http://dx.doi.org/10.1016/j.eurpolymj.2011.05.015

Marcos PM, Ascenso JR, Segurado MAP, Cragg PJ, Michel S, Hubscher-Bruder V, Arnaud-Neu F "Lanthanide cation binding properties of homooxacalixarene diethylamide derivatives" Supramolecular Chemistry 23, (1-2) 93-101 (2011). http://dx.doi.org/10.1080/10610278.2010.510562

Abrantes M, Bruno SM, Tomé C, Pillinger M, Gonçalves IS, Valente AA "Epoxidation of DL-limonene using an indenyl molybdenum(II) tricarbonyl complex as catalyst precursor" Catalysis Communications 15 (1), 64–67 (2011). http://dx.doi.org/10.1016/j.catcom.2011.08.015

Abrantes M, Gonçalves IS, Pillinger M, Vurchio C, Cordero FM, Brandi A "Molybdenum Oxide/Bipyridine Hybrid Material {[MoO3(bipy)][MoO3(H2O)]}n as Catalyst for the Oxidation of Secondary Amines to Nitrones" Tetrahedron Lett., 52, 7079–7082 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.10.079

Gomes CSB, Carabineiro SA, Gomes PT, Duarte MT, Lemos MANDA "Octahedral Co(III) Complexes of 2-(Phenylimino)pyrrolyl Ligands: Synthesis and Structural Characterisation" Inorganica Chimica Acta, 367 (1), 151-157 (2011). http://dx.doi.org/10.1016/j.ica.2010.12.032

Li L, Gomes CS, Gomes PT, Duarte MT, Fan Z "New tetradentate N,N,N,N-chelating α-diimine ligands and their corresponding zinc and nickel complexes: synthesis, characterisation and testing as olefin polymerisation catalysts" Dalton Trans., 40, (13) 3365-3380 (2011). http://dx.doi.org/10.1039/c0dt01308k

Li L, Gomes PT, Lemos MANDA, Lemos F, Fan Z "Polymerisation of Norbornene Catalysed by Highly Active Tetradentate Chelated α-Diimine Nickel Complexes" Macromolecular Chemistry and Physics, 212, 367-374, (2011). http://dx.doi.org/10.1002/macp.201000612

Yuan JC, Mei T, Gomes PT, Marques MM, Wang X, Liu Y, Miao C, Xie X "New Octahedral Bis-α-Diimine Nickel(II) Complexes Containing Chloro-substituted Aryl Groups: Synthesis, Characterization and Testing as Ethylene Polymerisation Catalysts" Journal of Organometallic Chemistry 696 (20): 3251-3256 (2011). http://dx.doi.org/10.1016/j.jorganchem.2011.07.009

Ventura AC, Fernandes CI, Saraiva MS, Nunes TG, Vaz PD, Nunes CD "Tuning the surface of mesoporous materials towards hydrophobicity effects in olefin epoxidation" Current Inorganic Chemistry 1, (2) 156-165 (2011). http://dx.doi.org/10.2174/10156

Silva NU, Fernandes CI, Nunes TG, Saraiva MS, Nunes CD, Vaz PD "Performance evaluation of mesoporous host materials in olefin epoxidation using Mo(II) and Mo(VI) active species – inorganic vs. hybrid matrix" Applied Catalysis A: General, 408, (1-2) 105-116 (2011). http://dx.doi.org/10.1016/j.apcata.2011.09.012

Antunes MA, Munhá RF, Alves LG, Schafer LL, Martins AM "Intramolecular Hydroamination Catalysis using trans-N,N'-Dibenzylcyclam Zirconium Complexes" Journal of Organometallic Chemistry 696, (1) 2-6, (2011). http://dx.doi.org/10.1016/j.jorganchem.2010.08.039

Barroso S, Adão P, Duarte MT, Meetsma A, Pessoa JC, Bouwkamp MW, Martins AM "Chiral Diamine bis(phenolate) Ti(IV) and Zr(IV) complexes: Syntheses, Structures and Reactivity" Eur. J. Inorg. Chem, 2011 (27): 4277–4290 (2011). http://dx.doi.org/10.1002/ejic.201100470

Sousa SCA, Fernandes AC "Rhenium-catalyzed deoxygenation of epoxides without adding any reducing agent" Tetrahedron Letters, 52 (51): 6960-6962 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.10.085

Tskhovrebov AG, Luzyanin KV, Dolgushin FM, da Silva MFCG, Pombeiro AJL, Kukushkin VY "Novel Reactivity Mode of Metal Diaminocarbenes: Palladium(II)-Mediated Coupling between Acyclic Diaminocarbenes and Isonitriles Leading to Dinuclear Species" Organometallics, 30 (12) 3362–3370 (2011). http://dx.doi.org/10.1021/om2002574

Tskhovrebov AG, Luzyanin KV, Kuznetsov ML, Sorokoumov VN, Balova IA, Haukka M, Kukushkin VY "Substituent R-dependent regioselectivity switch in nucleophilic addition of N-phenylbenzamidine to Pd(II)- and Pt(II)-complexed isonitrile RNC giving aminocarbene-like species" Organometallics, 30 (4) 863–874 (2011). http://dx.doi.org/10.1021/om101041g

Wanke R, Benisvy L, Kuznetsov ML, da Silva MF, Pombeiro AJ "Persistent Hydrogen-Bonded and Non-Hydrogen-Bonded Phenoxyl Radicals" Chemistry 17 (42); 11882–11892 (2011). http://dx.doi.org/10.1002/chem.201101509

Benisvy L, Wanke R, da Silva MFCG, Pombeiro AJL "A Dianionic Dinickel(II) Complex and Its Oxidised Phenoxyl Radical States" Eur. J. Inorg. Chem. 2011 (18) 2191–2796 (2011). http://dx.doi.org/10.1002/ejic.201100232

Fernandes RR, Lasri J, da Silva MFCG, Kirillov AM, Silva JAL, Fraústo da Silva JJR, Pombeiro AJL "New Fe(II) and Cu(II) complexes bearing azathia macrocycles: catalyst precursors for mild peroxidative oxidation of cyclohexane and 1-phenylethanol" European Journal of Inorganic Chemistry, 2011 (25) 3781-3790 (2011). http://dx.doi.org/10.1002/ejic.201100460

Fernandes RR, Lasri J, da Silva MFCG, Palavra AMF, da Silva JAL, Fraústo da Silva JJR, Pombeiro AJL "Oxadiazoline and Ketoimine Palladium(II) Complexes as Highly Efficient Catalysts for Suzuki–Miyaura Cross-Coupling Reactions in Supercritical Carbon Dioxide" Advanced Synthesis and Catalysis, 353, (7) 1153-1160 (2011). http://dx.doi.org/10.1002/adsc.201000909

Kopylovich MN, Lasri J, da Silva MFG, Pombeiro AJL "PdII-Promoted Single-Pot Template Transformations of Benzonitriles, Cyanoguanidine and Sodium Dicyanamide with the Formation of Symmetrical and Asymmetrical (1,3,5-Triazapentadienate)palladium(II) Complexes" Eur. J. Inorg. Chem. 2011 (3) 377–383 (2011). http://dx.doi.org/10.1002/ejic.201000898

Kopylovich MN, Mahmudov KT, da Silva MF, Kirillov AM, Pombeiro AJ. "Unusual shift of a nitro group in a phenylhydrazo-β-diketone" Dalton Trans. 40 (46): 12472-8 (2011). http://dx.doi.org/10.1039/c1dt11209k

Kopylovich MN, Mahmudov KT, Haukka M, Luzyanin KV, Pombeiro AJL "(E)-2-(2-(2-hydroxyphenyl)hydrazono)-1-phenylbutane-1,3-dione: tautomery and coordination to copper(II)" Inorganica Chimica Acta, 374 (1), 175-180 (2011). http://dx.doi.org/10.1016/j.ica.2011.02.094

Kopylovich MN, Nunes AC, Mahmudov KT, Haukka M, Mac Leod TC, Martins LM, Kuznetsov ML, Pombeiro AJ.

"Complexes of copper(II) with 3-(ortho-substituted phenylhydrazo)pentane-2,4-diones: syntheses, properties and catalytic activity for cyclohexane oxidation" Dalton Transactions, 40 (12), 2822-2836 (2011). http://dx.doi.org/10.1039/c0dt01527j

Kopylovich MN, Mahmudov KT, Guedes da Silva MFC, Figiel PJ, Karabach YY, Luznetsov ML, Luzyanin KV, Pombeiro AJL "Ortho-Hydroxyphenylhydrazo-β-Diketones: Tautomery, Coordination Ability, and Catalytic Activity of Their Copper(II) Complexes toward Oxidation of Cyclohexane and Benzylic Alcohols" Inorg. Chem. 50 (3), 918-931. http://dx.doi.org/10.1021/ic101516k

Lasri J, Mac Leod TCO, Pombeiro AJL "Oxadiazoline and ketoimine palladium(II) complexes supported on a chitosan membrane and their catalytic activity for the microwave-assisted Suzuki–Miyaura cross-coupling in water" Appl. Catal. A: Gen., 397, 94–102 (2011). http://dx.doi.org/10.1016/j.apcata.2011.02.019

Lasri J, Rodríguez MJF, Guedes da Silva MFC, Smoleński P, Kopylovich MN, Fraústo da Silva JJR, Pombeiro AJL. "Microwave Synthesis of Bis(tetrazolato)-PdII Complexes with PPh3 and Water-soluble 1,3,5-triaza-7-phosphaadamantane (PTA). The First Example of C-CN Bond Cleavage of Propionitrile by a PdII Centre" Journal of Organometallic Chemistry, 696 (22): 3513-3520, (2011). http://dx.doi.org/10.1016/j.jorganchem.2011.07.047

Mahmudov KT, Kopylovich MN, Luzyanin KV, Archana M, Guedes da Silva MFC, Andre V, Pombeiro AJL "Structural and thermal properties of three cyanosubstituted azoderivatives of β-diketones" Journal of Molecular Structure, 992 (1-3): 72-76 (2011). http://dx.doi.org/10.1016/j.molstruc.2011.02.045

Mahmudov KT, Rahimov RA, Babanly MB, Hasanov PQ, Pashaev FG, Gasanov AG, Kopylovich MN, Pombeiro AJL "Tautomery and acid–base properties of some azoderivatives of benzoylacetone" Journal of Molecular Liquids, 162 (2), 84-88 (2011). http://dx.doi.org/10.1016/j.molliq.2011.06.005

da Silva JLF, Galvao AC, Ferreira AP, Galvão AM, Dias AR, Gomes PT, Salema MS "Effect of ancillary ligands in the hapticity of the pyrrolyl ligand in [Ti(pyrrolyl)(NMe2)(x)Cl3-x] (x=0, 1, 2, 3) complexes" J. Organom. Chem, 695 (10-11) 1533-1540 (2010). http://dx.doi.org/10.1016/j.jorganchem.2010.03.007

Cabrita I, Fernandes AC "A novel efficient and chemoselective method for the reduction of nitriles using the system silane/oxo-rhenium complexes" Tetrahedron 67, (42) 8183-8186 (2011). http://dx.doi.org/10.1016/j.tet.2011.08.015

Antunes AM, Novais DA, da Silva JL, Santos PP, Oliveira MC, Beland FA, Marques MM. "Synthesis and oxidation of 2-hydroxynevirapine, a metabolite of the HIV reverse transcriptase inhibitor nevirapine" Org. Biomol. Chem. 9 (22) 7822-7835 (2011). http://dx.doi.org/10.1039/c1ob06052j

Charneira C, Godinho AL, Oliveira MC, Pereira SA, Monteiro EC, Marques MM, Antunes AM "Reactive aldehyde metabolites from the anti-HIV drug abacavir: amino acid adducts as possible factors in abacavir toxicity" Chem. Res. Toxicol, 24 (12): 2129-2141 (2011). http://dx.doi.org/10.1021/tx200337b

Ferreira da Silva JL, Ferreira AP, Marques MM, Harjivan SG, Minas da Piedade MF, Duarte MT "Effect of C–H…X interactions (X = O, S, π) in the supramolecular arrangements of 3-ferrocenyl-methoxybenzo[b]thiophene isomers" Cryst Eng Comm, 13, 1638-1645 (2011). http://dx.doi.org/10.1039/C0CE00434K

Brotas G, Farinhas J, Ferreira Q, Morgado J, Charas A. "Nanostructured layers of a new cross-linkable poly(3-hexylthiophene) in organic photovoltaic cells" Synthetic Metals, 162, (23): 2052-2058 (2012). http://dx.doi.org/10.1016/j.synthmet.2012.10.007

Rocha A, Carvalho T, Vidinha P, Lourenço NMT "Synthesis and properties of novel room temperature choline carboxylate zwitterionic ionic liquids as potential electrolytes" Chempluschem, 77, 1106-1111 (2012). http://dx.doi.org/10.1002/cplu.201200247

Suresh D, Gomes CSB, Gomes PT, Di Paolo RE, Maçanita AL, Calhorda MJ, Charas A, Morgado J, Duarte MT "Syntheses and photophysical properties of new iminopyrrolyl boron complexes and their application in efficient single-layer non-doped OLEDs prepared by spin coating" Dalton Trans., 41, 8502-8505 (2012). http://dx.doi.org/10.1039/C2DT30487B

Alves LG, Hild F, Munhá RF, Veiros LF, Dagorne S, Martins AM "Synthesis and structural characterization of novel cyclam-based zirconium complexes and their use in the controlled ROP of rac-lactide: access to cyclam-

functionalized polylactide materials" Dalton Trans., 41, (47): 14288-98 (2012). http://dx.doi.org/10.1039/c2dt31133j

Antunes MA, Alves LG, Namorado S, Ascenso JR, Veiros LF, Martins AM. "Hydride Abstraction from [MCpBz(CO)3H] (M = Mo, W; CpBz = C5(CH2Ph)5): New Cationic Complexes Stabilized by η5:η2-C5H4:C6H5 Bonding of the Pentabenzylcyclopentadienyl Ligand" Organometallics, 31, (12): 4387-4396 (2012). http://dx.doi.org/10.1021/om300070m

Alves LG, Martins AM. "Cyclam functionalization through isocyanate insertion in Zr-N bonds" Inorg Chem., 51, (1): 10-2 (2012). http://dx.doi.org/10.1021/ic201750y

Li L. Lopes PS, Rosa V, Figueira CA, Lemos MANDA, Duarte MT, Aviles T, Gomes PT. "Synthesis and structural characterisation of (aryl-BIAN)copper(I) complexes and their application as catalysts for the cycloaddition of azides and alkynes" Dalton Trans., 41, 5144-5154 (2012). http://dx.doi.org/10.1039/C2DT11854H

Adao P, Kuznetsov ML, Barroso S, Martins AM, Avecilla F, Pessoa JC. "Amino Alcohol-Derived Reduced Schiff Base VIVO and VV Compounds as Catalysts for Asymmetric Sulfoxidation of Thioanisole with Hydrogen Peroxide" Inorg Chem., 51 (21): 11430-11449 (2012). http://dx.doi.org/10.1021/ic301153p

Amarante TR, Neves P, Tomé C, Abrantes M, Valente AA, Paz FA, Pillinger M, Gonçalves IS. "An octanuclear molybdenum(VI) complex containing coordinatively bound 4,4'-di-tert-butyl-2,2'-bipyridine, [Mo8O22(OH)4(di-tBu-bipy)4]: synthesis, structure, and catalytic epoxidation of bio-derived olefins" Inorg Chem., 51 (6): 3666-76 (2012). http://dx.doi.org/10.1021/ic202640a

Gomes AC, Bruno SM, Tomé C, Valente AA, Pillinger M, Abrantes M, Gonçalves IS. "Synthesis and characterization of CpMo(CO)3(CH2–pC6H4–CO2CH3) and its inclusion compounds with methylated cyclodextrins. Applications in olefin epoxidation catalysis" Journal of Organometallic Chemistry, in press (2012). http://dx.doi.org/10.1016/j.jorganchem.2012.12.019

Tomé C, Oliveira MC, Pillinger M, Gonçalves IS, Abrantes M. "Use of MoO2Cl2(DMF)2 as a precursor for molybdate promoted hydrolysis of phosphoester bonds" Dalton Trans., in press (2012). http://dx.doi.org/10.1039/C2DT32734A

Moneo A, Carvalho MFNN, Telo JP "Dicyanoaromatic radical anions as mixed valence species" J. Phys. Org. Chem., 25: 559-565 (2012). http://dx.doi.org/10.1002/poc.2905

Cerdeira AC, Afonso ML, Santos IC, Pereira LCJ, Coutinho JT, Rabaca S, Simao D, Henriques RT, Almeida M. "Synthesis, structure and physical properties of transition metal bis 4-cyanobenzene-1,2-dithiolate complexes [M(cbdt)2]z– (M = Zn, Co, Cu, Au, Ni, Pd, z = 0, 1, 2)" Polyhedron, 44 (1): 228-237 (2012). http://dx.doi.org/10.1016/j.poly.2012.07.010

Espa D, Pilia L, Marchiò L, Artizzu F, Serpe A, Mercuri ML, Simão D, Almeida M, Pizzotti M, Tessore F, Deplano P. "Mixed-ligand Pt(II) dithione-dithiolato complexes: influence of the dicyanobenzodithiolato ligand on the second-order NLO properties" Dalton Trans., 41, 3485-3493 (2012). http://dx.doi.org/10.1039/C2DT11956K

Costa AI, Prata JV. "Substituted p-phenylene ethynylene trimers as fluorescent sensors for nitroaromatic explosives" Sensors and Actuactors: Chemical B, 161 (1): 251-260 (2012). http://dx.doi.org/10.1016/j.snb.2011.10.027

Costa AI, Pinto HD, Ferreira LFV, Prata JV. "Solid-State Sensory Properties of Calix-Poly(phenylene ethynylene)s toward Nitroaromatic Explosives" Sensors and Actuators: Chemical B, 161, (1): 702-713 (2012). http://dx.doi.org/10.1016/j.snb.2011.11.017

Barata PD., Costa AI, Prata JV. "Calix[4]arene-carbazole-containing polymers: Synthesis and properties" Reactive and Functional Polymers, 72 (9): 627-634 (2012). http://dx.doi.org/10.1016/j.reactfunctpolym.2012.06.006

Chay RS, Luzyanin KV, Kukushkin VY, Guedes da Silva MFC, Pombeiro AJL. "Novel palladium-aminocarbene species derived from metal-mediated coupling of isonitriles and 1,3-diiminoisoindoline: synthesis and catalytic application in Suzuki–Miyaura cross-coupling" Organometallics, 31 (6): 2379-2387 (2012). http://dx.doi.org/10.1021/om300020j

Chay RS, Luzyanin KV. "Evaluation of catalytic properties of aminocarbene species derived from the integration between 3-iminoisoindolin-1-ones and palladium-bound isonitriles in Suzuki–Miyaura cross-coupling" Inorg. Chim. Acta, 380: 322–327 (2012). http://dx.doi.org/10.1016/j.ica.2011.09.047

Rocha BGM, Wanke R, da Silva MFCG, Luzyanin KV, Martins LMDRS, Smolenski P, Pombeiro AJL. "Reactivity of bulky tris(phenylpyrazolyl)methanesulfonate copper(I) complexes towards small unsaturated molecules" J.

Organomet Chemistry, 714: 47-52 (2012). http://dx.doi.org/10.1016/j.jorganchem.2012.03.022

Kandhavelu M, Paturu L, Mizar A, Mahmudov KT, Kopylovich MN, Karp M, Yli-Harja O, Pombeiro AJL, Ribeiro AS. "Synthesis, characterization and antimicrobial activity of arylhydrazones of methylene active compounds" Pharmaceutical Chemistry Journal 46 (3): 157-164 (2012). http://dx.doi.org/10.1007/s11094-012-0751-y

Kopylovich MN, Mac Leod TC, Haukka M, Amanullayeva GI, Mahmudov KT, Pombeiro AJ. "Aquasoluble iron(III)-arylhydrazone-b-diketone complexes: structure and catalytic activity for the peroxidative oxidation of C5-C8 cycloalkanes" J Inorg Biochem, 115: 72-77 (2012). http://dx.doi.org/10.1016/j.jinorgbio.2012.05.008

Mac Leod TCO, Kopylovich MN, Guedes da Silva MFC, Mahmudov KT, Pombeiro AJL. "Copper(II) complexes of arylhydrazones of β-diketones immobilized on Zn–Al-layered double hydroxides as effective recyclable catalysts for peroxidative oxidation of alkanes". Applied Catalysis A: General 439-440: 15-23 (2012). http://dx.doi.org/10.1016/j.apcata.2012.06.032

Kopylovich MN, Gajewska MJ, Mahmudov KT, Kirillova MV, Figiel PJ, Guedes da Silva MFC, Gil-Hernández B, Sanchiz J, Pombeiro AJL. "Copper(II) complexes with a new carboxylic-functionalized arylhydrazone of β-diketone as effective catalysts for the acid-free oxidations" New J. Chem., 36 (8), 1646-1654 (2012). http://dx.doi.org/10.1039/C2NJ40210F

Mahmudov KT, Guedes da Silva MFC, Glucini M, Renzi M, Gabriel KCP, Kopylovich MN, Sutradhar M, Marchetti F, Pettinari C, Zamponi S, Pombeiro AJL. "Water-soluble heterometallic copper(II)-sodium complex comprising arylhydrazone of barbituric acid as a ligand" Inorganic Chemistry Communications, 22: 187-189 (2012). http://dx.doi.org/10.1016/j.inoche.2012.06.008

Ma Z, Maharramov AM, Aliyev IA, Aliyeva IN, Kopylovich MN, Amanullayeva GI, Mahmudov KT, Pombeiro AJL. "New arylhydrazones of β-diketones and their optical and thermal properties". Journal of Molecular Structure, 1019: 16-20 (2012). http://dx.doi.org/10.1016/j.molstruc.2012.03.054

Kuznik W, Kopylovich MN, Amanullayeva GI, Pombeiro AJL, Reshak AH, Mahmudov KT, Kityk IV "Role of tautomerism and solvatochromism in UV–VIS spectra of arylhydrazones of β-diketones" Journal of Molecular Liquids, 171: 11-15 (2012). http://dx.doi.org/10.1016/j.molliq.2012.03.023

Mizar A, Guedes da Silva MFC, Kopylovich MN, Mukherjee S, Mahmudov KT, Pombeiro AJL. "Water-soluble copper(II) complexes with a sulfonic-functionalized arylhydrazone of b-diketone and their application in peroxidative allylic oxidation of cyclohexene". Eur. J. Inorg Chem., 2012 (13): 2305-2313 (2012). http://dx.doi.org/10.1002/ejic.201101361

Mahmudov KT, Kopylovich MN, Kuznetsov ML, Maharramov AM, Aliyeva RA, Aliyev IA, Azizov AA, Pombeiro AJL "Thermodynamics of Dissociation of ortho-Hydroxyphenylhydrazo-β-diketones and of their Complexation with Copper(II) in Aqueous-ethanol solutions". Journal of Solution Chemistry, 41 (3): 491-502 (2012). http://dx.doi.org/10.1007/s10953-012-9816-5

Sousa SCA, Bernardo JR, Fernandes AC. "Highly efficient oxidation of benzyl alcohols using the catalytic system sulfoxide/oxo-complexes". Tetrahedron Letters, 53 (46): 6205-6208 (2012). http://dx.doi.org/10.1016/j.tetlet.2012.08.145

Sousa SCA, Bernardo JR, Romão CC, Fernandes AC. "Highly efficient rhenium-catalyzed deoxygenation of sulfoxides without adding any reducing agent", Tetrahedron, 68 (39): 8194-8197 (2012). http://dx.doi.org/10.1016/j.tet.2012.07.071

Gaeta C, Talotta C, Farina F, Teixeira FA, Marcos PM, Ascenso JR, Neri P. "Alkylammonium cation complexation into the narrow cavity of dihomooxacalix[4]arene macrocycle" J. Org. Chem., 77 (22): 10285–10293 (2012). http://dx.doi.org/10.1021/jo3019945

Ferreira JA, Sánchez-Coronilla A, Togashi DM, Ferreira H, Ascenso JR, Costa SM. "Electrophilic Reactivity of Tetrabromorhodamine 123 is Bromine Induced: Convergent Interpretation through Complementary Molecular Descriptors", J. Phys. Chem. A, 116 (48): 11938–11945 (2012). http://dx.doi.org/10.1021/jp307461m

Silva NU, Nunes TG, Saraiva MS, Shalamzari MS, Vaz PD, Monteiro OC, Nunes CD. "Photocatalytic degradation of rhodamine B using Mo heterogeneous catalysts under aerobic conditions" Applied Catalysis B: Environmental, 113-114: 180-191 (2012). http://dx.doi.org/10.1016/j.apcatb.2011.11.036

Antunes AM, Sidarus M, Novais DA, Harjivan SG, Santos PP, Ferreira da Silva JL, Beland FA, Marques MM. "Oxidation of 2-Hydroxynevirapine, a Phenolic Metabolite of the Anti-HIV Drug Nevirapine: Evidence for an Unusual Pyridine Ring Contraction" Molecules 17 (3): 2616-2627 (2012). http://dx.doi.org/10.3390/molecules17032616

Wanke R, Novais DA, Harjivan SG, Marques MM, Antunes AM. "Biomimetic oxidation of aromatic xenobiotics: synthesis of the phenolic metabolites from the anti-HIV drug Efavirenz" Org. Biomol. Chem., 10 (23): 4554-4561 (2012). http://dx.doi.org/10.1039/c2ob25212k

Caixas U, Antunes AM, Marinho AT, Godinho AL, Grilo NM, Marques MM, Oliveira MC, Branco T, Monteiro EC, Pereira SA. "Evidence for nevirapine bioactivation in man: searching for the first step in the mechanism of nevirapine toxicity". Toxicology, 301 (1-3): 33-39 (2012). http://dx.doi.org/10.1016/j.tox.2012.06.013

Charneira C, Grilo NM, Pereira SA, Godinho AL, Monteiro EC, Marques MM, Antunes AM. "N-terminal valine adduct from the anti-HIV drug abacavir in rat hemoglobin as evidence for abacavir metabolism to a reactive aldehyde in vivo". Br. J. Pharmacol. 167 (6): 1353-1361 (2012). http://dx.doi.org/10.1111/j.1476-5381.2012.02079.x

REQUIMTE - FCT - Universidade Nova de Lisboa

Book Chapters

A. Viegas, A. L. Macedo, E. J. Cabrita "Ligand based nuclear magnetic resonance screening techniques", in Ligand Macromolecule Interactions in drug discovery, Methods in Molecular Biology, edited by Ana Cecília A. Roque, Humana Press USA, vol. 572, 81-100, (2010).

Scientific Papers

Aldrey A; Nunez C; Garcia V, Bastida R, Lodeiro C, Macias A "Anion sensing properties of new colorimetric chemosensors based on macrocyclic ligands bearing three nitrophenylurea groups" Tetrahedron, 66, 47: 9223-9230 (2010). http://dx.doi.org/10.1016/j.tet.2010.09.054

Pinheiro, AV; Parola, AJ; Baptista, PV, Lima JC "pH Effect on the Photochemistry of 4-Methylcoumarin Phosphate Esters: Caged-Phosphate Case Study" J. Phys Chem A 114, 12795-803 (2010). http://dx.doi.org/10.1021/jp103045u

Pereira M, Leal CR, Parola AJ, Scheven UM "Reversible Photorheology in Solutions of Cetyltrimethylammonium Bromide, Salicylic Acid, and trans-2,4,4′-Trihydroxychalcone" Langmuir, 26 16715-16721 (2010). http://dx.doi.org/10.1021/la102267d

Estevao MS, Carvalho LC, Ribeiro D, Couto D, Freitas M, Gomes A, Ferreira LM, Fernandes E, Marques MM. "Antioxidant activity of unexplored indole derivatives: Synthesis and screening" Eur J Med Chem 45: 4869-4878 (2010). http://dx.doi.org/10.1016/j.ejmech.2010.07.059

Carvalho LR, Corvo MC, Enugala R, Marques MM, Cabrita EJ "Application of HR-MAS NMR in the solid-phase synthesis of a glycopeptide using Sieber amide resin" Magnetic Resonance in Chemistry 48: 323-330 (2010). http://dx.doi.org/10.1002/mrc.2583

Andrade MM, Barros MT, Pinto RC "Approach to the Valorization of Carbohydrates as Raw Materials by Microwave-Assisted Neat 1,3- Dipolar Cycloaddition" Synthetic Communications 40: 855-860 (2010). http://dx.doi.org/10.1080/00397910903019959

Martins JG, Pinto RM, Gameiro P, Barros MT, Soares HMVM "Aqueous Equilibrium and Solution Structural Studies of the Interaction of N,N'-bis(4-imidazolymethyl)etylenediamine with Ca(II), Cd(II), Co(II), Cu(II), Mg(II), Mn(II), Ni(II), Pb(II) and Zn(II) Metal Ions" Journal of Solution Chemistry 39 (8): 1153-1167 (2010). http://dx.doi.org/10.1007/s10953-010-9569-y

Teixeira J, Silva AR, Branco LC, Afonso CAM, Freire C "Asymmetric alkene epoxidation by Mn(III)salen catalyst in ionic liquids" Inorganica Chimica Acta 363 (13): 3321-3329 (2010). http://dx.doi.org/10.1016/j.ica.2010.06.018

Duarte FJS, Cabrita EJ, Frenking G, Santos AG "Asymmetric Intramolecular Aldol Reactions of Substituted 1,7-Dicarbonylic Compounds. A Mechanistic Study" J Org Chem 75: 2546-2555 (2010). http://dx.doi.org/10.1021/jo100026h

Branco PS, Raje VP, Dourado J, Gordo J "Catalyst-free aziridination and unexpected homologation of aziridines from imines" Org Biomol Chem 8: 2968-2974 (2010). http://dx.doi.org/10.1039/c001894e

Gavara R, Petrov V, Pina F “Characterization of the 4 '-hydroxynaphthoflavylium network of chemical reactions” Photochem Photobiol Sci 9: 298-303 (2010). http://dx.doi.org/10.1039/b9pp00035f

Bonifacio VDB, Gonzalez-Bello C, Rzepa HS, Prabhakar S, Lobo AM “Chiral Aziridination of Olefins Using a Chiral Sulfinamide as the Nitrogen Source” Synlett 2010 (1): 145-149 (2010). http://dx.doi.org/10.1055/s-0029-1218545

da Silva MS, Vao ER, Temtem M, Mafra L, Caldeira J, Aguiar-Ricardo A, Casimiro T “Clean synthesis of molecular recognition polymeric materials with chiral sensing capability using supercritical fluid technology. Application as HPLC stationary phases” Biosens Bioelectron 25 (7): 1742-1747 (2010). http://dx.doi.org/10.1016/j.bios.2009.12.023

Rosa V, Santos CIM, Welter R, Aullon G, Lodeiro C, Aviles T “Comparison of the Structure and Stability of New alpha-Diimine Complexes of Copper(I) and Silver(I): Density Functional Theory versus Experimental” Inorg Chem 49, 8699-8708 (2010). http://dx.doi.org/10.1021/ic100450y

Rondao R, de Melo JSS, Bonifacio VDB, Melo MJ “Dehydroindigo, the Forgotten Indigo and Its Contribution to the Color of Maya Blue” Journal of Physical Chemistry A 114 (4): 1699-1708 (2010). http://dx.doi.org/10.1021/jp907718k

Restani RB, Correia VG, Bonifacio VDB, Aguiar-Ricardo A “Development of functional mesoporous microparticles for controlled drug delivery” J of Supecriticalr Fluids 55, 333-339 (2010). http://dx.doi.org/10.1016/j.supflu.2010.08.007

Andrade MM, Barros MT “Fast Synthesis of N-Acylhydrazones Employing a Microwave Assisted Neat Protocol” Journal of Combinatorial Chemistry 12 (2): 245-247 (2010). http://dx.doi.org/10.1021/cc9001444

Gavara R, Laia CA, Parola AJ, Pina F “Formation of a leuco spirolactone from 4-(2-carboxyphenyl)-7-diethylamino-4'-dimethylamino-1-benzopyrylium: design of a phase-change thermochromic system based on a flavylium dye.” Chemistry 16 (26): 7760-7766 (2010). http://dx.doi.org/10.1002/chem.200903482

Figueire VBC, Esque AG, Varala R, Gonzalez-Bello C, Prabhakar S, Lobo AM “Functional desymmetrization of 1,3-dioximes for the obtention of 1,2,3-hetero trisubstituted carbocycles” Tetrahedron Letters 51: 2029-2031 (2010). http://dx.doi.org/10.1016/j.tetlet.2010.02.048

Leydet Y, Parola AJ, Pina F “Hydroxypyridinechromene and Pyridinechalcone: Two Coupled Photochromic Systems” Chemistry 16: 545-555 (2010). http://dx.doi.org/10.1002/chem.200901884

Carrera GVSM, Afonso CAM, Branco LC “Interfacial Properties, Densities, and Contact Angles of Task Specific Ionic Liquids” Journal of Chemical and Engineering Data 55 (2): 609-615 (2010). http://dx.doi.org/10.1021/je900502s

Serbanovic A, Petrovski Z, Manic M, Marques CS, Carrera G, Branco LC, Afonso CAM, da Ponte MN “Melting behaviour of ionic salts in the presence of high pressure CO2” Fluid Phase Equilibria 294: 121-130 (2010). http://dx.doi.org/10.1016/j.fluid.2010.03.015

Carvalho LC, Estevao MS, Ferreira LM, Fernandes E, Marques MMB “A new insight on the hypochlorous acid scavenging mechanism of tryptamine and tryptophan derivatives” Bioorg Med Chem Lett 20: 6475-6478 (2010). http://dx.doi.org/10.1016/j.bmcl.2010.09.067

Martins S, Branco PS, de la Torre MC, Sierra MA, Pereira A “New Methodology for the Synthesis of 3-Substituted Coumarins via Palladium-Catalyzed Site- Selective Cross-Coupling Reactions” Synlett 2010 (19): 2918-2922 (2010). http://dx.doi.org/10.1055/s-0030-1259014

Goodfellow BJ, Duarte I, Macedo AL, Volkman BF, Nunes SG, Moura I, Markley JL, Moura JJG “An NMR structural study of nickel-substituted rubredoxin” J Biol Inorg Chem 15: 409-420 (2010). http://dx.doi.org/10.1007/s00775-009-0613-6

Morgado L, Saraiva IH, Louro RO, Salgueiro CA “Orientation of the axial ligands and magnetic properties of the hemes in the triheme ferricytochrome PpcA from G. sulfurreducens determined by paramagnetic NMR” Febs Letters 584: 3442-3445 (2010). http://dx.doi.org/10.1016/j.febslet.2010.06.043

Petrovski Z, Martins BMR, Afonso CAM “Short synthesis of methylenecyclopentenones by intermolecular Pauson-Khand reaction of allyl thiourea” Tetrahedron Letters 51, (26): 3356-3359 (2010). http://dx.doi.org/10.1016/j.tetlet.2010.04.025

Vitoriano BC, Carvalho LCR, Estevao MS, Sekera MH, Marques MMB “A Simple Route Toward New Clomiphene Metabolites” Synlett 2010 (5): 753-756 (2010). http://dx.doi.org/10.1055/s-0029-1219383

Gomes R, Albuquerque RQ, Pina F, Parola AJ, De Cola L "Supramolecular host-guest flavylium-loaded zeolite L hybrid materials: network of reactions of encapsulated 7,4 '-dihydroxyflavylium" Photochem Photobiol Sci. 9: 991-995 (2010). http://dx.doi.org/10.1039/c0pp00022a

Barros MT, Petrova KT, Singh RP "Synthesis and biodegradation studies of new copolymers based on sucrose derivatives and styrene" European Polymer Journal 46 (5): 1151-1157 (2010). http://dx.doi.org/10.1016/j.eurpolymj.2010.02.002

Carrera GVSM, Frade RFM., Aires-de-Sousa J, Afonso CAM, Branco LC "Synthesis and properties of new functionalized guanidinium based ionic liquids as non-toxic versatile organic materials" Tetrahedron 66: 8785-8794 (2010). http://dx.doi.org/10.1016/j.tet.2010.08.040

Barros MT, Petrova KT, Singh RP "Synthesis of Hydrophilic and Amphiphilic Acryl Sucrose Monomers and Their Copolymerisation with Styrene, Methylmethacrylate and alpha- and beta-Pinenes" Int J Mol Sci. 11 (4): 1792-1807 (2010). http://dx.doi.org/10.3390/ijms11041792

Bonifacio VDB, Morgado J, Scherf U. "Synthesis of Thiosulfonate-Bridged Bromofluorene Endcapping Reagents" Synlett 2010 (9): 1333-1336 (2010). http://dx.doi.org/10.1055/s-0029-1219905

Pinto LFV, Justino GC, Vieira AJSC, Prabhakar S, Lobo AM "Thermal rearrangement of an N-hydroxyimidazole thiocarbamoyl derivative as a simple entry into the 4-thioimidazole motif" Arkivoc 2010: 17-23 (2010).

Morgado L, Bruix M, Pessanha M, Londer YY, Salgueiro CA "Thermodynamic Characterization of a Triheme Cytochrome Family from Geobacter sulfurreducens Reveals Mechanistic and Functional Diversity" Biophys J 99, 293-301 (2010). http://dx.doi.org/10.1016/j.bpj.2010.04.017

Enugala R, Carvalho LCR, Marques MMB "Towards Glucosamine Building Blocks: Regioselective One-Pot Protection and Deallylation Procedures" Synlett 2010 (18): 2711-2716 (2010). http://dx.doi.org/10.1055/s-0030-1259001

Morgado L, Paixão VB, Salgueiro CA, Bruix M "Backbone, side chain and heme resonance assignments of the triheme cytochrome PpcA from Geobacter sulfurreducens" Biomol. NMR Assign, 5 (1): 113-116 (2011). http://dx.doi.org/10.1007/s12104-010-9280-3

Dantas JM, Saraiva IH, Morgado L, Silva MA, Schiffer M, Salgueiro CA, Louro RO "Orientation of the axial ligands and magnetic properties of the hemes in the cytochrome c(7) family from Geobacter sulfurreducens determined by paramagnetic NMR" Dalton Trans 40, (47): 12713-12718 (2011). http://dx.doi.org/10.1039/c1dt10975h.

Rui M. Almeida, Carlos F. G. C. Geraldes, Sofia R. Pauleta, José J. G. Moura "Gd(III) Chelates as NMR Probes of Protein-Protein Interactions. Case Sudy: Rubredoxin and Cytochrome c3" Inorg. Chem., 50, 10600-10607 (2011). http://dx.doi.org/10.1021/ic200858c

Bonifacio VDB; Kumar RP; Prabhakar S, Lobo AM "O-Substituted N-oxy arylsulfinamides and sulfonamides in Michael reactions", Arkivoc, Part 10: 266-U1 (2011).

Correia VG, Bonifacio VD; Raje VP; Casimiro T, Moutinho G, da Silva CL, Pinho MG, Aguiar-Ricardo A "Oxazoline-based antimicrobial oligomers: synthesis by CROP using supercritical CO2" Macromol. Biosci. 11, (8): 1128-1137 (2011). http://dx.doi.org/10.1002/mabi.201100126

Lopes JM, Petrovski Z, Bogel-Lukasik R, Bogel-Lukasik E "Heterogeneous palladium-catalyzed telomerization of myrcene with glycerol derivatives in supercritical carbon dioxide: a facile route to new building blocks", Green Chem. 13: 2013-2016 (2011). http://dx.doi.org/10.1039/C1GC15313G

Ramos S, Almeida RM, Moura JJG, Aureliano M "Implications of oxidovanadium(IV) binding to actin" Journal of Inorganic Biochemistry 105 (6): 777-783 (2011). http://dx.doi.org/10.1016/j.jinorgbio.2011.02.010

Gawande MB, Branco PS "An efficient and expeditious Fmoc protection of amines and amino acids in aqueous media" Green Chem. 13 3355-3359 (2011). http://dx.doi.org/10.1039/C1GC15868F

Gordo J, Avo J, Parola AJ, Lima JC, Pereira A, Branco PS "Convenient Synthesis of 3-Vinyl and 3-Styryl Coumarins" Org. Lett. 13 (19) 5112-5115 (2011). http://dx.doi.org/10.1021/ol201983u.

Lopes LC, Roman B, Medeiros MA, Mukhopadhyay A, Utrilla P, Gálvez J, Mauriño SG, Moltiva V, Lourenço A, Feliciano AS "Cernumidine and isocernumidine, new type of cyclic guanidine alkaloids from Solanum cernuum" Tetrahedron Letters 52 (48) 6392–6395 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.09.060

Estevao MS, Carvalho LC, Ferreira LM, Fernandes E, Marques MMB "Analysis of the antioxidant activity of an indole library: cyclic voltammetry versus ROS scavenging activity" Tetrahedron Letters 52 (1) 101–106 (2011). http://dx.doi.org/10.1016/j.tetlet.2010.10.172

Carvalho LCR, Fernandes E, Marques MMB "Developments Towards Regioselective Synthesis of 1,2-Disubstituted Benzimidazoles" Chem. Eur. J., 17 (45), 12544-12555 (2011). http://dx.doi.org/10.1002/chem.201101508

Barros MT, Petrova KT, Correia-da-Silva P, Potewar TM "Library of Mild and Economic Protocols for the Selective Derivatization of Sucrose under Microwave Irradiation" Green Chem. 13, 1897-1906 (2011). http://dx.doi.org/10.1039/C1GC15228A

Barros MT, Phillips AMF "Organocatalyzed Synthesis of Tertiary α-Hydroxyphosphonates by a Highly Regioselective Modified Pudovik Reaction" Eur. J. Org. Chem., IYC Special Issue: Women in Chemistry, 2011 (20-21) 4028-4036 (2011). http://dx.doi.org/10.1002/ejoc.201100308

Barros MT, Mouquinho AI, Petrova KT, Saavedra MD, Sotomayor JC "Fast synthesis employing a microwave assisted neat protocol of new monomers potentially useful for the preparation of PDLC films" Cent. Eur. J. Chem., 9 (4), 557-566 (2011). http://dx.doi.org/10.2478/s11532-011-0046-2

Mouquinho A, Saavedra M, Maiau A, Petrova K, Barros MT, Figueirinhas JL, Sotomayor J "Films based on new methacrylate monomers: synthesis, characterisation and electro-optical properties" Mol. Cryst. Liq. Cryst., 542 132-140 (2011). http://dx.doi.org/10.1080/15421406.2011.570154

Martins JG, Barros MT, Pinto RM, Soares HMVM "Cadmium(II), Lead(II), and Zinc(II) Ions Coordination of N,N'-(S,S)Bis[1-carboxy-2-(imidazol-4yl)ethyl]ethylenediamine: Equilibrium and Structural Studies" J. of Chem. Eng. Data, 56 (3) 398-405 (2011). http://dx.doi.org/10.1021/je1007718

Lanham AB, Carvalheira M, Rodrigues AM, Cardoso VV, Benoliel MJ, Barros MT, Morgado MJ, Soares HM, Lemos PC, Reis MA "Ethylenediamine-N,N'-diglutaric acid (EDDG) as a promising biodegradable chelator: quantification, complexation and biodegradation" J Environ Sci Health A Tox Hazard Subst Environ Eng, 46 (6), 553-559 (2011). http://dx.doi.org/10.1080/10934529.2011.562805

Pinto RM, Dias AA, Costa ML, Rodrigues P, Barros MT, Ogden JS, Dyke JM "Thermal decomposition of methyl 2-Azidopropionate studied by UV photoelectron spectroscopy and matrix isolation IR spectroscopy: heterocyclic intermediate vs. imine formation" J. Phys. Chem. A, 115 (30), 8447–8457 (2011). http://dx.doi.org/10.1021/jp2036845

Duarte FJS, Bakalova SM, Cabrita EJ, Santos AG "Lewis Acid Catalyzed Reactions of Chiral Imidazolidinones and Oxazolidinones: Insights on the Role of the Catalyst" Journal of Organic Chemistry, 76, (17) 6997-7004 (2011). http://dx.doi.org/10.1021/jo201318f

Viegas A, Manso J, Corvo MC, Marques MM, Cabrita EJ "Binding of ibuprofen, ketorolac and diclofenac to COX-1 and COX-2 studied by saturation transfer difference NMR" J. Med. Chem., 54, 8555-8562 (2011). http://dx.doi.org/10.1021/jm201090k

Soares da Silva M, Nobrega F, Cabrita EJ, Aguiar-Ricardo A, Casimiro T "Development of molecularly imprinted co-polymeric devices for controlled drug delivery of flufenamic acid using supercritical fluid technology" J. of Supercritical Fluids, 58, 150-157 (2011). http://dx.doi.org/10.1016/j.supflu.2011.05.010

Cruz C, Cabrita EJ, Queiroz JA "Screening nucleotide binding to amino acid-coated supports by surface plasmon resonance and nuclear magnetic resonance" Anal. Bioanal. Chem., 401, (3) 983-993 (2011). http://dx.doi.org/10.1007/s00216-011-5124-y

Cruz C, Cabrita EJ, Queiroz JA "Analysis of nucleotides binding to chromatography supports provided by nuclear magnetic resonance spectroscopy" J Chromatogr A, 1218 3559-64 (2011). http://dx.doi.org/10.1016/j.chroma.2011.03.055

Viegas A, Manso J, Nobrega FL, Cabrita EJ "Saturation-Transfer Difference (STD) NMR – A simple and fast method for ligand screening and characterization of protein binding" J. Chem. Educ. 88 (7) 990-994 (2011). http://dx.doi.org/10.1021/ed101169t

Oliveira J, Petrov V, Parola AJ, Pina F, Azevedo J, Teixeira N, Brás NF, Fernandes PA, Mateus N, Ramos MJ, de Freitas V "Chemical Behavior of Methylpyranomalvidin-3-O-glucoside in Aqueous Solution Studied by NMR and UV-

Visible Spectroscopy" J. Phys. Chem. B, 115, 1538-1545 (2011). http://dx.doi.org/10.1021/jp110593c

Diniz AM, Pinheiro C, Petrov V, Parola AJ, Pina F "Synthesis and Characterization of a Symmetric Bis-7-hydroxyflavylium Containing a Methyl Viologen Bridge" Chemistry 17, (23) 6359-6368 (2011). http://dx.doi.org/10.1002/chem.201003726

Avó J, Parola AJ, Lima JC, Pina F, Cunha-Silva L "Phase Transition Thermochromism Based on C-H Acidity of 4-Alkylflavylium Compounds in Pluronic F-127". J. Mater. Chem. 21, 16628-16637 (2011). http://dx.doi.org/10.1039/C1JM13348A

Swager TM, Schnorr JM "A One-Pot Route to 3-Vinyl Coumarins" Synfacts, 2011 (12), 1310-1310 (2011). http://dx.doi.org/10.1055/s-0031-1289429

Rosatella AA, Afonso CAM, Branco LC "Oxidation of Cyclohexene to trans-1,2-Cyclohexanediol Promoted by p-Toluenesulfonic Acid without Organic Solvents" J. Chem. Educ. 88 (7) 1002-1003 (2011). http://dx.doi.org/10.1021/ed1006772

Branco A, Branco LC, Pina F "Electrochromic and magnetic ionic liquids" Chem. Commu. 47, 2300-2302 (2011). http://dx.doi.org/10.1039/C0CC03892J

Costa E, de-Carvalho J, Casimiro T, da Silva CL, Cidade MT; Aguiar-Ricardo A, "Tailoring thermoresponsive microbeads in supercritical carbon dioxide for biomedical applications" Journal of Supercritical Fluids, 56, (3), 292-298 (2011). http://dx.doi.org/10.1016/j.supflu.2010.10.039

Merino EG, Atlas S, Raihane M, Belfkira A, Lahcini M, Hult A, Dionisio M, Correia, NT "Molecular dynamics of poly(ATRIF) homopolymer and poly(AN-co-ATRIF) copolymer investigated by dielectric relaxation spectroscopy" European Polymer Journal, 47 (7) 1429-1446 (2011). http://dx.doi.org/10.1016/j.eurpolymj.2011.04.006

Siopa F, Pereira AS, Ferreira LM, Matilde Marques M, Branco PS. "Synthesis of catecholamine conjugates with nitrogen-centered bionucleophiles" Bioorg. Chem., 44: 19-24 (2012). http://dx.doi.org/10.1016/j.bioorg.2012.05.002

Universidade do Porto

Book Chapters

Martins D, Costa N, Ferra J, Cruz P, Mendes A, Magalhães F, Carvalho LHC. "Characterisation of urea-formaldehyde resins using 13C NMR spectroscopy", in ECOWOOD 2010-Minimizing the environmental impact of the forest products industries, edited by Fernando Caldeira, Edições Universidade Fernando Pessoa (Porto), pp. 203-209 (ISBN 978-989-643-083-2).

Scientific Papers

Nunes A, Podinovskaia M, Leite A, Gameiro P, Zhou T, Ma Y, Kong X, Schaible UE, Hider RC, Rangel M. "Fluorescent 3-hydroxy-4-pyridinone hexadentate iron chelators: intracellular distribution and the relevance to anti-mycobacterial properties" J. Biol. Inorg. Chem., 15 (6): 861-877 (2010). http://dx.doi.org/10.1007/s00775-010-0650-1

Peres I, Rocha S, Pereira MC, Coelho M, Rangel M, Ivanova G. "NMR structural analysis of epigallocatechin gallate loaded polysaccharide nanoparticles", Carbohydrate Polymers, 82 (3): 861–866 (2010). http://dx.doi.org/10.1016/j.carbpol.2010.06.007

Silva AMG, Leite A, Andrade M, Gameiro P, Brandão P, Felix V, de Castro B, Rangel M. "Microwave-assisted synthesis of 3-hydroxy-4-pyridinone/naphthalene conjugates. Structural characterization and selection of a fluorescent ion sensor" Tetrahedron, 66 (44): 8544-8550 (2010). http://dx.doi.org/10.1016/j.tet.2010.08.065

Helguera AM, Rodríguez-Borges JE, CaamañoO, García-Mera X, González MP, Cordeiro MNDS. "Design, Synthesis and Evaluation of Antineoplastic Activity of Novel Carbocyclic Nucleosides" Molecular Informatics, 29 (3): 213-231 (2010). http://dx.doi.org/10.1002/minf.200900033

Rodríguez-Borges JE, García-Mera X, Balo MC, Brea J, Caamaño O, Fernández F, López C, Loza MI, Nieto MI. "Synthesis and pharmacological evaluation of novel 1,3,8- and 1,3,7,8-substituted xanthines as adenosine receptor antagonists" Bioorg Med Chem., 18 (5): 2001-9 (2010). http://dx.doi.org/10.1016/j.bmc.2010.01.028

Nieto MI, Balo MC, Brea J, Caamaño O, Fernández F, García-Mera X, López C, Loza MI, Rodríguez-Borges JE, Vidal B. "Synthesis and Pharmacological Evaluation of Novel Substituted-9-deazaxanthines as A_2B Receptor Antagonists" Eur. J. Med. Chem., 45 (7): 2884-2892 (2010). http://dx.doi.org/10.1016/j.ejmech.2010.03.011

Sousa CAD, Vale MLC, Rodríguez-Borges JE, García-Mera X. "Phosphorylation of 2-azabicyclo[2.2.1]hept-5-ene and 2-hydroxy-2-azabicyclo[2.2.1]hept-5-ene systems: synthesis and mechanistic study" New J. Chem., 34, 2546-2551 (2010). http://dx.doi.org/10.1039/C0NJ00239A

da Costa JF, Caamano O, Fernandez F, Garcia-Mera X, Midon P, Rodriguez-Borges JE. "Synthesis of methyl (±)-3,5-bis(substitutedmethyl)pyrrolidine-2-carboxylates: A convenient approach to proline-mimetics" Tetrahedron, 66 (34): 6797-6805 (2010). http://dx.doi.org/10.1016/j.tet.2010.06.053

Matos J, Vale N, Collins MS, Gut J, Rosenthal PJ, Cushion MT, Moreira R, Gomes P. "PRIMACENES: novel non-cytotoxic primaquine-ferrocene conjugates with anti-Pneumocystis carinii activity" Med. Chem. Commun., 1, 199-201 (2010). http://dx.doi.org/10.1039/C0MD00082E

Quezada E, Viña D, Delogu G, Borges F, Santana L, Uriarte E. "Synthesis of Carbocyclic Pyrimidine Nucleosides Using the Mitsunobu Reaction: O2- vs. N1-Alkylation" Helv. Chim. Acta, 93 (2): 309-313 (2010). http://dx.doi.org/10.1002/hlca.200900242

Paiva-Martins F, Fernandes J, Santos V, Silva L, Borges F, Rocha S, Belo L, Santos-Silva A "Powerful protective role of 3,4-dihydroxyphenylethanol elenolic acid dialdehyde against erythrocyte oxidative induced hemolysis" J. Agric. Food Chem., 58 (1): 135-140 (2010). http://dx.doi.org/10.1021/jf9031052

Alcaro S, Gaspar A, Ortuso F, Milhazes N, Orallo F, Uriarte E, Yáñez M, Borges F. "Chromone-2- and -3-carboxylic acids inhibit differently monoamine oxidases A and B" Bioorg Med Chem Lett., 20 (9): 2709-12 (2010). http://dx.doi.org/10.1016/j.bmcl.2010.03.081

Reis B, Martins M, Barreto B, Milhazes N, Garrido EM, Silva P, Garrido J, Borges F. "Structure-property-activity relationship of phenolic acids and derivatives. Protocatechuic acid alkyl esters" J Agric Food Chem., 58 (11): 6986-93 (2010). http://dx.doi.org/10.1021/jf100569j

Cortez J, Vorobieva E, Gralheira D, Osório I, Soares L, Vale N, Pereira E, Gomes P, Franco R. "Bionanoconjugates of tyrosinase and peptide-derivatised gold nanoparticles for biosensing of phenolic compounds" Journal of Nanoparticle Research, 13 (3): 1101-13 (2011). http://dx.doi.org/10.1007/s11051-010-0099-8

Azevedo J, Fernandes I, Faria A, Oliveira J, Fernandes A, de Freitas V, Mateus N. "Antioxidant properties of anthocyanidins, anthocyanidin-3-glucosides and respective portisins" Food Chemistry, 119, (2): 518-523 (2010). http://dx.doi.org/10.1016/j.foodchem.2009.06.050

Nave F, Teixeira N, Mateus N, de Freitas V. "The fate of flavanol-anthocyanin adducts in wines: Study of their putative reaction patterns in the presence of acetaldehyde" Food Chemistry, 121, (4): 1129-1138 (2010). http://dx.doi.org/10.1016/j.foodchem.2010.01.060

Fernandes I, Faria A, Azevedo J, Soares S, Calhau C, de Freitas V, Mateus N. "Influence of Anthocyanins, Derivative Pigments and Other Catechol and Pyrogallol-Type Phenolics on Breast Cancer Cell Proliferation" J. Agric. Food Chem., 58 (6): 3785-3792 (2010). http://dx.doi.org/10.1021/jf903714z

Cruz L, Brás NF, Teixeira N, Mateus N, Ramos MJ, Dangles O, De Freitas V. "Vinylcatechin dimers are much better copigments for anthocyanins than catechin dimer procyanidin b3", J. Agric. Food Chem. 58, (5): 3159-3166 (2010). http://dx.doi.org/10.1021/jf9037419

Sousa A, Mateus N, Silva AMS, Vivas N, Nonier MF, Pianet I, de Freitas V. "Isolation and Structural Characterization of Anthocyanin-furfuryl Pigments" J Agric Food Chem 58, (9), 5664-69 (2010). http://dx.doi.org/10.1021/jf1000327

Oliveira J, Azevedo J, Silva AMS, Teixeira N, Cruz L, Mateus N, de Freitas V. "Pyranoanthocyanin Dimers: A New Family of Turquoise Blue Anthocyanin-Derived Pigments Found in Port Wine" J Agric Food Chem. 58, (8), 5154-5159 (2010). http://dx.doi.org/10.1021/jf9044414

Brás NF, Gonçalves R, Fernandes PA, Mateus N, Ramos MJ, de Freitas V. "Understanding the binding of procyanidins to pancreatic elastase by experimental and computational methods" Biochemistry 49, (25): 5097-5108 (2010). http://dx.doi.org/10.1021/bi100410q

He JR, Oliveira J, Silva AMS, Mateus N, De Freitas V. "Oxovitisins: A New Class of neutral pyranone-anthocyanin derivatives in red wines" J Agric. Food Chem. 58, (15), 8814-8819 (2010). http://dx.doi.org/10.1021/jf101408q

He J, Carvalho AR, Mateus N, De Freitas V. “Spectral features and stability of oligomeric pyranoanthocyanin-flavanol pigments isolated from red wines” J. Agric. Food Chem., 58 (16): 9249-9258 (2010). http://dx.doi.org/10.1021/jf102085e

Brás NF, Gonçalves R, Mateus N, Fernandes PA, Ramos MJ, de Freitas V. “Inhibition of pancreatic elastase by polyphenolic compounds” J. Agric. Food Chem., 58 (19), 10668–10676 (2010). http://dx.doi.org/10.1021/jf1017934

Kontoudakis N, Esteruelas M, Fort F, Canals JM, de Freitas V, Zamora F. “Influence of the heterogeneity of grape phenolic maturity on wine composition and quality” Food Chemistry, 124 (3): 767-774 (2011). http://dx.doi.org/10.1016/j.foodchem.2010.06.093

Fernandes A, Sousa A, Mateus N, Cabral M, de Freitas V. “Analysis of phenolic compounds in cork from Quercus suber L. by HPLC-DAD/ESI-MS” Food Chemistry 125 (4): 1398-1405 (2011). http://dx.doi.org/10.1016/j.foodchem.2010.10.016

Gonçalves R, Mateus N, de Freitas V. “Inhibition of α-amylase activity by condensed tannins” Food Chemistry 125 (2): 665-672 (2011). http://dx.doi.org/10.1016/j.foodchem.2010.09.061

Nave F, Petrov V, Pina F, Teixeira N, Mateus N, de Freitas V. “Thermodynamic and kinetic properties of a red wine pigment: catechin-(4,8)-malvidin-3-O-glucoside” J Phys Chem. B,. 114 (42): 13487-96 (2010). http://dx.doi.org/10.1021/jp104749f

Cruz L, Petrov V, Teixeira N, Mateus N, Pina F, de Freitas V. “Establishment of the chemical equilibria of different types of pyranoanthocyanins in aqueous solutions: evidence for the formation of aggregation in pyranomalvidin-3-O-coumaroylglucoside-(+)-catechin” J Phys Chem. B., 114 (41): 13232-40 (2010). http://dx.doi.org/10.1021/jp1045673

Gonçalves R, Mateus N, de Freitas V. “Study of the interaction of pancreatic lipase with procyanidins by optical and enzymatic methods” J Agric. Food Chem., 58, (22): 11901-11906 (2010). http://dx.doi.org/10.1021/jf103026x

Azevedo J, Teixeira N, Oliveira J, de Freitas V, Mateus N. “Effect of sugar acylation on the antioxidant properties of Vitis vinifera red grape malvidin-3-glucoside” Int. J. Food Sci. Technol. 46 (2): 343-349 (2011). http://dx.doi.org/10.1111/j.1365-2621.2010.02497.x

Brougham DF, Ivanova G, Gottschalk M, Collins DM, Eustace AJ, O’Connor R, Havel J. “Artificial Neural Networks for Classification in Metabolomic Studies of Whole Cells Using 1H Nuclear Magnetic Resonance” Journal of Biomedicine and Biotechnology, 2011 Article ID 158094 (8 pages) (2011). http://dx.doi.org/10.1155/2011/158094

Ivanova G, Simeonova M, Cabrita EJ, Rangel M “NMR Insight into the Supramolecular Structure of Daunorubicin Loaded Polymer Nanoparticles” J. Phys. Chem. B, 115, 902-909 (2011). http://dx.doi.org/10.1021/jp109738e

Christova N, Tuleva B, Cohenb R, Ivanova G, Stoevd G, Stoilova-Disheva M, Stoineva I. “Chemical Characterization and Physical and Biological Activities of Rhamnolipids Produced by Pseudomonas aeruginosa BN10” Zeitschrift fur Naturforschung - Section C, 66 (7-8): 394-402 (2011). PMID: 21950164

Markova N, Ivanova G, Enchev V, Simeonova M. “Tacticity of poly(butyl-α-cyanoacrylate) chains in nanoparticles: NMR spectroscopy and DFT calculations” Structural Chemistry, 23 (3): 815-824 (2011). http://dx.doi.org/10.1007/s11224-011-9928-3

Leite A, Silva AMG, Nunes A, Andrade M, Sousa C, Cunha-Silva L, Gameiro P, de Castro B, Rangel M. “Novel tetradentate chelators derived from 3-hydroxy-4-pyridinone units: synthesis, characterization and aqueous solution properties” Tetrahedron, 67 (22): 4009-4016 (2011). http://dx.doi.org/10.1016/j.tet.2011.04.035

Silva AMG, Leite A, Gonzalez P, Domingues MRM, Gameiro P, de Castro B, Rangel M. “Use of a porphyrin platform and 3,4-HPO chelating units to synthesize ligands with N4 and O4 coordination sites” Tetrahedron 67, (40): 7821-7828 (2011). http://dx.doi.org/10.1016/j.tet.2011.07.063

Gonçalves R, Mateus N, De Freitas V. “Influence of carbohydrates on the interaction of procyanidin B3 with trypsin” J Agric Food Chem., 59, (21): 11794-11802 (2011). http://dx.doi.org/10.1021/jf203060s

Gonçalves R, Mateus N, Pianet I, Laguerre M, de Freitas V. “Mechanisms of tannin-induced trypsin inhibition: a molecular approach” Langmuir 27 (21): 13122-9 (2011). http://dx.doi.org/10.1021/la202280c

de Freitas V, Mateus N “Formation of pyranoanthocyanins in red wines: a new and diverse class of anthocyanin

derivatives" Anal. Bioanal. Chem. 401 (5): 1463-73 (2011). http://dx.doi.org/10.1007/s00216-010-4479-9

Oliveira J, Mateus N, Rodriguez-Borges JE, Cabrita EJ, Silva AMS, de Freitas V. "Synthesis of a new pyranoanthocyanin dimer linked through a methyl-methine bridge" Tetrahedron Lett. 52, (23): 2957-2960 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.03.125

He JR, Silva AMS, Mateus N, de Freitas V. "Oxidative formation and structural characterisation of new alpha-pyranone (lactone) compounds of non-oxonium nature originated from fruit anthocyanins" Food Chemistry 127, (3), 984-992 (2011). http://dx.doi.org/10.1016/j.foodchem.2011.01.069

Oliveira J, Mateus N, de Freitas V. "Synthesis of a new bluish pigment from the reaction of a methylpyranoanthocyanin with sinapaldehyde" Tetrahedron Lett. 52, (16): 1996-2000 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.02.079

Oliveira J, Petrov V, Parola AJ, Pina F, Azevedo J, Teixeira N, Brás NF, Fernandes PA, Mateus N, Ramos MJ, de Freitas V. "Chemical behavior of methylpyranomalvidin-3-O-glucoside in aqueous solution studied by NMR and UV-visible spectroscopy" J Phys Chem B., 115, (6): 1538-1545 (2011). http://dx.doi.org/10.1021/jp110593c

Paiva-Martins F, Rodrigues V, Calheiros R, Marques MP. "Characterization of antioxidant olive oil biophenols by spectroscopic methods" J Sci Food Agric, 91 (2): 309-314 (2011). http://dx.doi.org/10.1002/jsfa.4186

García-Mera X, Rodríguez-Borges JE, Vale MLC, Alves MJ. "Highly diastereoselective synthesis of 2-azabicyclo[2.2.1]hept-5-ene derivatives: Bronsted acid catalyzed aza-Diels-Alder reaction between cyclopentadiene and imino-acetates with two chiral auxiliaries" Tetrahedron 67 (37), 7162-7172 (2011). http://dx.doi.org/10.1016/j.tet.2011.06.097

Brito RO, Silva SG, Fernandes RM, Marques EF, Enrique-Borges J, do Vale ML. "Enhanced interfacial properties of novel amino acid-derived surfactants: Effects of headgroup chemistry and of alkyl chain length and unsaturation" Colloids Surf B Biointerfaces 86 (1): 65-70 (2011). http://dx.doi.org/10.1016/j.colsurfb.2011.03.017

Oliveira J, Mateus N, Rodriguez-Borges JE, Cabrita EJ, Silva AMS, de Freitas V "Synthesis of a new pyranoanthocyanin dimer linked through a methyl-methine bridge", Tetrahedron Letters, 52 (23): 2957-2960 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.03.125

Menezes JC, Kamat SP, Cavaleiro JA, Gaspar A, Garrido J, Borges F. "Synthesis and antioxidant activity of long chain alkyl hydroxycinnamates" Eur J Med Chem., 46 (2): 773-7 (2011). http://dx.doi.org/10.1016/j.ejmech.2010.12.016

Gaspar A, Reis J, Fonseca A, Milhazes N, Viña D, Uriarte E, Borges F. "Chromone 3-phenylcarboxamides as potent and selective MAO-B inhibitors" Bioorg Med Chem Lett. 21 (2): 707-9 (2011). http://dx.doi.org/10.1016/j.bmcl.2010.11.128

Gaspar A, Teixeira F, Uriarte E, Milhazes N, Melo A, Cordeiro MN, Ortuso F, Alcaro S, Borges F. "Towards the discovery of a novel class of monoamine oxidase inhibitors: structure-property-activity and docking studies on chromone amides" ChemMedChem. 6 (4): 628-32 (2011). http://dx.doi.org/10.1002/cmdc.201000452

Cagide F, Reis J, Gaspar A, Borges F. "Accelerating lead optimization of chromone carboxamide scaffold throughout microwave-assisted organic synthesis" Tetrahedron Letters, 52 (48): 6446-6449 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.09.095

Matos MJ, Vazquez-Rodriguez S, Borges F, Santana L, Uriarte E. "Synthesis of 3-arylcoumarins via Suzuki-cross-coupling reactions of 3-chlorocoumarin" Tetrahedron Letters, 52, (11): 1225-1227 (2011). http://dx.doi.org/10.1016/j.tetlet.2011.01.048

Markova N, Ivanova G, Enchev V, Simeonova M. "Tacticity of poly(butyl-α-cyanoacrylate) chains in nanoparticles: NMR spectroscopy and DFT calculations", Structural Chemistry, 23 (3):815–824 (2012). http://dx.doi.org/10.1007/s11224-011-9928-3

Georgiev L, Chochkova M, Totseva I, Seizova K, Marinova E, Ivanova G, Ninova M, Najdenski H, Milkova T. "Anti-tyrosinase, antioxidant and antimicrobial activities of hydroxycinnamoylamides" Med. Chem. Res. 2012. http://dx.doi.org/10.1007/s00044-012-0419-x

Cardoso ICS, Amorim AL, Queirós C, Lopes SC, Gameiro P, de Castro B, Rangel M, Silva AMG. "Microwave-Assisted Synthesis and Spectroscopic Properties of 4-Substituted Rosamine Fluorophores and Naphthyl Analogues", Eur. J. Org. Chem., 2012: 5810-5817 (2012). http://dx.doi.org/10.1002/ejoc.201200783

Lopes S, Simeonova M, Gameiro P, Rangel M, Ivanova G. "Interaction of 5-fluorouracil loaded nanoparticles with DMPC liposomes used as cellular membrane models", J. Phys. Chem. B, 116 (1): 667-675 (2012). http://dx.doi.org/10.1021/jp210088n

Queirós C, Silva AMG, Lopes SC, Ivanova G, Gameiro P, Rangel M. "A novel fluorescein-based dye containing a catechol chelating unit to sense iron(III)", Dyes and Pigments, 93: 1447-55 (2012). http://dx.doi.org/10.1016/j.dyepig.2011.10.010

Carneiro AP, Rodriguez O, Macedo EA. "Solubility of monosaccharides in ionic liquids - Experimental data and modelling", Fluid Phase Equilib. 314: 22-28 (2012). http://dx.doi.org/10.1016/j.fluid.2011.10.011

Carneiro AP, Rodriguez O, Macedo EA. "Solubility of xylitol and sorbitol in ionic liquids - Experimental data and modeling", J. Chem. Thermodyn. 55: 184-192 (2012). http://dx.doi.org/10.1016/j.jct.2012.05.020

Peres I, Rocha S, Loureiro JA, Pereira MC, Ivanova G, Coelho M., "Carbohydrate particles as protein carriers and scaffolds: physic-chemical characterization and collagen stability", Journal of Nanoparticles Research, 14: 1144 (2012). http://dx.doi.org/10.1007/s11051-012-1144-6

Barbosa JV, Oliveira F, Moniz J, Magalhães FD, Bastos MMSM. "Synthesis and characterization of allyl fatty acid derivative as coalescing agent for latexes", Journal of the American Oil Chemists Society, 89 (12): 2215-2226 (2012). http://dx.doi.org/10.1007/s11746-012-2114-y

Barbosa JV, Veludo E, Moniz J, Magalhães FD, Bastos MMSM. "Synthesis and characterization of acrylic fatty acid derivative", Eur. J Lipid Sci. Technol., 114: 1175–1182 (2012). http://dx.doi.org/10.1002/ejlt.201100388

Costa C, Alves A, Pinto PR, Sousa RA, da Silva EAB, Reis RL, Rodrigues AE. "Characterization of ulvan extracts to assess the effect of different steps in extraction procedure" Carbohydrate Polymers, 88 (2): 537-546 (2012). http://dx.doi.org/10.1016/j.carbpol.2011.12.041

Silva ME, Lemos LT, Bastos MM, Nunes OC, Cunha-Queda AC. "Recovery of humic-like substances from low quality composts", Bioresour Technol., 128C: 624-632 (2012). http://dx.doi.org/10.1016/j.biortech.2012.11.013

Nave F, Brás NF, Cruz L, Teixeira N, Mateus N, Ramos MJ, Di Meo F, Trouillas P, Dangles O, De Freitas V. "Influence of a flavan-3-ol substituent on the affinity of anthocyanins (pigments) toward vinylcatechin dimers and proanthocyanidins (copigments)", J. Phys. Chem.B, 116 (48): 14089-14099 (2012). http://dx.doi.org/10.1021/jp307782y

Fernandes I, Nave F, Gonçalves R, de Freitas V, Mateus N. "On the bioavailability of flavanols and anthocyanins: flavanol-anthocyanin dimers", Food Chem., 135 (2): 812-818 (2012). http://dx.doi.org/10.1016/j.foodchem.2012.05.037

Soares S, Mateus N, de Freitas V. "Carbohydrates inhibit salivary proteins precipitation by condensed tannins", J. Agric. Food Chem., 60 (15): 3966-3972 (2012). http://dx.doi.org/10.1021/jf3002747

Fernandes I, de Freitas V, Reis C, Mateus N. "A new approach on the gastric absorption of anthocyanins", Food Funct., 3 (5): 508-516 (2012). http://dx.doi.org/10.1039/c2fo10295a

Sousa A, Mateus N, de Freitas V. "A novel reaction mechanism for the formation of deoxyanthocyanidins", Tetrahedron Lett., 53 (10): 1300-1303 (2012). http://dx.doi.org/10.1016/j.tetlet.2012.01.006

Sousa A, Fernandes A, Mateus N, De Freitas V. "Synthesis and structural characterization of oaklin-catechins", J. Agric. Food Chem., 60 (6): 1528-1534 (2012). http://dx.doi.org/10.1021/jf204408p

Algarra M, Campos BB, Rodríguez-Borges JE, Sanchez FG, Lopez-Romero JM, da Silva JCGE. "Niclosamide quantification in methyl-β-cyclodextrin after derivatization to aminoniclosamide", J. Incl. Phenom. Macrocycl. Chem. 72 (1-2): 89-94 (2012). http://dx.doi.org/10.1007/s10847-011-9945-2

Sousa CAD, Vale MLC, Rodriguez-Borges JE, Garcia-Mera X. "Structural analysis of three methyl N-phosphorylated 5,6-dihydroxy-2-azabicyclo[2.2.1]heptane-3-carboxylates" Journal of Molecular Structure 1007: 31-35 (2012). http://dx.doi.org/10.1016/j.molstruc.2011.09.041

Sousa CAD, Rizzo-Aguiar F, Vale MLC, García-Mera X, Caamaño O, Rodríguez-Borges JE. "A route to selective functionalization of polyhydroxypyrrolidines", Tetrahedron Letters 53 (9): 1029-1032 (2012). http://dx.doi.org/10.1016/j.tetlet.2011.12.037

Sousa CAD, Vale MLC, Garcia-Mera X, Rodríguez-Borges JE. "1,3- versus 1,4-[π4+π2] Cycloadditions between methyl glyoxylate oxime and cyclopentadiene or

cyclopentene" Tetrahedron 68 (6): 1682-1687 (2012). http://dx.doi.org/10.1016/j.tet.2011.12.073

Grou CP, Francisco T, Rodrigues TA, Freitas MO, Pinto MP, Carvalho AF, Domingues P, Wood SA, Rodríguez-Borges JE, Sá-Miranda C, Fransen M, Azevedo JE. "Identification of ubiquitin-specific protease 9X (USP9X) as a deubiquitinase acting on ubiquitin-peroxin 5 (PEX5) thioester conjugate" J Biol Chem., 287 (16): 12815-27 (2012). http://dx.doi.org/10.1074/jbc.M112.340158

Silva SG, Fernandes RF, Marques EF, do Vale MLC. "Serine-Based Bis-quat Gemini Surfactants: Synthesis and Micellization Properties", Eur. J. Org. Chem., 2012 (2): 345–352 (2012). http://dx.doi.org/10.1002/ejoc.201101118

Calejo MT, Kjoniksen A-L, Marques EF, Araújo MJ, Sande SA, Nystrom B. "Interactions between ethyl(hydroxyethyl) cellulose and lysine-based surfactants in aqueous media" European Polymer Journal, 48 (9): 1622-1631 (2012). http://dx.doi.org/10.1016/j.eurpolymj.2012.06.009

Viveiros MLF, Freitas VLS, Vale N, Gomes JRB, Gomes P, da Silva MDMCR "Synthesis and thermochemical study of quinoxaline N-oxides: enthalpies of dissociation of the N-O bond" J Phys Org Chem, 25 (5): 420-426 (2012). http://dx.doi.org/10.1002/poc.1932

Matos J, da Cruz FP, Cabrita É, Gut J, Nogueira F, do Rosário VE, Moreira R, Rosenthal PJ, Prudêncio M, Gomes P. "Novel potent metallocenes against liver stage malaria" Antimicrob Agents Chemother. 56 (3): 1564-70 (2012). http://dx.doi.org/10.1128/AAC.05345-11

Pérez BC, Teixeira C, Figueiras M, Gut J, Rosenthal PJ, Gomes JR, Gomes P. "Novel cinnamic acid/4-aminoquinoline conjugates bearing non-proteinogenic amino acids: towards the development of potential dual action antimalarials" Eur J Med Chem., 54: 887-899 (2012). http://dx.doi.org/10.1016/j.ejmech.2012.05.022

Vale-Costa S, Vale N, Matos J, Tomás A, Moreira R, Gomes P, Gomes MS. "Peptidomimetic and organometallic derivatives of primaquine active against Leishmania infantum" Antimicrob Agents Chemother., 56 (11): 5774-81 (2012). http://dx.doi.org/10.1128/AAC.00873-12

Teixeira J, Soares P, Benfeito S, Gaspar A, Garrido J, Murphy MP, Borges F. "Rational discovery and development of a mitochondria-targeted antioxidant based on cinnamic acid scaffold", Free Radic Res., 46 (5): 600-11 (2012). http://dx.doi.org/10.3109/10715762.2012.662593

Costa Lima S, Rodrigues V, Garrido J, Borges F, Kong Thoo Lin P, Cordeiro da Silva A. "In vitro evaluation of bisnaphthalimidopropyl derivatives loaded into pegylated nanoparticles against Leishmania infantum protozoa", Int J Antimicrob Agents, 39 (5): 424-30 (2012). http://dx.doi.org/10.1016/j.ijantimicag.2012.01.003

Gaspar A, Reis J, Kachler S, Paoletta S, Uriarte E, Klotz K-N, Moro S, Borges F. "Discovery of novel A(3) adenosine receptor ligands based on chromone scaffold", Biochem Pharmacol., 84 (1): 21-29 (2012). http://dx.doi.org/10.1016/j.bcp.2012.03.007

Gaspar A, Reis J, Matos MJ, Uriarte E, Borges F. "In search for new chemical entities as adenosine receptor ligands: development of agents based on benzo-γ-pyrone skeleton" Eur J Med Chem., 54, 914-8 (2012). http://dx.doi.org/10.1016/j.ejmech.2012.05.033

Viña D, Matos MJ, Ferino G, Cadoni E, Laguna R, Borges F, Uriarte E, Santana L. "8-Substituted 3-arylcoumarins as potent and selective MAO-B inhibitors: synthesis, pharmacological evaluation, and docking studies" ChemMedChem. 7 (3), 464-70 (2012). http://dx.doi.org/10.1002/cmdc.201100538

Garrido J, Garrido EM, Borges F. "Studies on the Food Additive Propyl Gallate: Synthesis, Structural Characterization, and Evaluation of the Antioxidant Activity", J. Chem. Educ., 89 (1): 130–133 (2012). http://dx.doi.org/10.1021/ed900025s

Garrido J, Gaspar A, Garrido EM, Miri R, Tavakkoli M, Pourali S, Saso L, Borges F, Firuzi O. "Alkyl esters of hydroxycinnamic acids with improved antioxidant activity and lipophilicity protect PC12 cells against oxidative stress", Biochimie., 94 (4): 961-7 (2012). http://dx.doi.org/10.1016/j.biochi.2011.12.015

Matos MJ, Gaspar A, Borges F, Uriarte E, Santana L. "Improved synthesis of 3-(aminoaryl)coumarins" Org. Prep. Proc. Int., 44 (6): 522-526 (2012). http://dx.doi.org/10.1080/00304948.2012.730937

Reis J, Oliveira C, Milhazes N, Viña D, Borges F. "Exploring nitrostyrene as a scaffold for a new class a of monoamine oxidase inhibitors" Lett Drug Design Discovery, 9 (10): 958-961 (2012).

Garrido EM, Santos M, Silva P, Cagide F, Garrido J, Borges F. "Host-guest complexes of phenoxy alkyl acid herbicides and cyclodextrins. MCPA and β-cyclodextrin" J. Environ.

Science and Health, Part B, 47 (9): 869-875 (2012). http://dx.doi.org/10.1080/03601234.2012.693867

Annex 3

Supported Research Projects

Biological Chemistry – Biological Engineering

PTDC/QUI-BIQ/113880/2009/ Studies on the structure/activity relationship of AI-2, a bacterial signalling molecule for inter-species communication (2011-2014)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget: 137 K€

PTDC/EBB-EBI/113727/2009/ PhytoLac - Engineered Lactococcus lactis for the optimized production of nutraceutical plant-derived polyphenols (2011-2014)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget: 159 K€

PTDC/QUI-BIQ/115298/2009/ Identification of plant extracts with protective action against bacterial enterotoxins belonging to AB5 group: cholera toxin, heat labile toxin from Eshcherichia coli and shiga toxin (dysentery) (2011-2014)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget: 73 K€

PTDC/QUI-BIQ/114904/2009/ Solution structure and mode of action of the dimeric bacteriocin Lcn972 (2011-2014)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget: 78 K€

PTDC/QUI-QUI/117105/2010/ The effect of divalent cations on G-Quadruplex formation and stability in genes related to neurodegenerative processes (2012-2015)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget: 78 K€

PTDC/BIA-PRO/117523/2010 Molecular mechanisms that orchestrate a two-electron reduction step coupled with protonation in redox enzymes that contain chains of single electron redox co-factors (2012-2015)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget: 138 K€

PTDC/QUI-BIQ/117440/2010 Redox necklaces: functional characterization of a multidomain polyheme cytochrome (2012-2015)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget 99 K€

PTDC/BIA-PRO/120949/2010 A molecular insight into the respiratory alternative complex III (2012-2015)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget 144 K€

PTDC/CVT/116499/2010 Lactation and milk production in Goat (Capra hircus): identifying molecular markers underlying adaptation to seasonal weight loss (2012-2015)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget 141 K€

PTDC/AAC-CLI/119100/2010 Soil function profiling during fungal bioremediation: integrated bio-geochemical and meta-proteomics assessment (2012-2015)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget 185 K€

PTDC/QUI-QUI/120982/2010 Creating value from bio-wastes: suberin extraction and biotransformation in biocompatible ionic liquids aiming on novel biomaterials and compounds (2012-2015)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget 87 K€

International Early Career Scientist Program of the Howard Hughes Medical Institute HHMI 55007436; Inter-species cell-cell signalling: its role in bacteria consortia (2012-2017)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)

PTDC/BIA-PRO/109796/2009 Insights into novel bacterial cytochrome c peroxidases from pathogenic bacteria, Neisseria gonorrhoeae and Escherichia coli.
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL Budget: 192 K€

PTDC/AGR-PRO/112340/2009 Ligand-binding stereospecificity of grapevine dirigent proteins: chiral induction for a new generation of fungicides.
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL Budget: 184 K€

PTDC/QUI-QUI/114236/2009, Sistemas paramagnéticos foto-induzidos estudados por Ressonância Magnética Nuclear. Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 73 K€.

PTDC/QUI-QUI/112597/2009 NANOLIGHT – Nanosystems for delivery of caged compounds
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 123 k€.

PTDC/SAU-IMU/111806/2009 Small immunoactive peptidoglycan (siPGN) derivatives to modulate an host inflammatory response. Instituto de Tecnologia Química e Biológica (ITQB/UNL) and Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 160 K€

MIT-Pt/BS-BB/0014/2008 Structural and functional study of the proteins mediating electron transfer between microorganisms and solid substrates with relevance for bio-energy production.
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL

PTDC/CTM/099452/2008 Smart Dendrimers
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 102 k€.

PTDC/QUI-BIQ/117799/2010/ Protein interaction with CO Releasing Molecules (CORM) (2012-2015)
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 150 K€

PTDC/EQU-EPR/104554/2008 The best of two worlds: Ionic liquids as Active Pharmaceutical Ingredients
Instituto de Tecnologia Química e Biológica (ITQB/UNL)
Budget: 111 k€

PTDC/BIA-PRO/098071/2008 Proteins with heterometalic centers involved in stress response
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL

PTDC/SAU-FCF/102958/2008 Implications of Amphetamine Psychostimulants Abuse in Brain Aging
Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares - Porto (ICETA-Porto/UP)
Budget: 200 k€.

PTDC/SAU-OSM/101437/2008 Development and Application of P-Glycoprotein Inducers for the Prophylaxis and Therapeutics of Xenobiotics Toxicity.
Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares - Porto (ICETA-Porto/UP)
Budget: 197 k€.

PTDC/BIA-PRO/098882/2008 A novel bacterial system involved in copper tolerance
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 186 k€.

PTDC/QUI-QUI/098892/2008 Study of intermolecular interactions in alternative solvents: A NMR based contribution to sustainable chemistry
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 198 k€.

QREN 2008/1433 Discovery and development of compounds for colon cancer therapy (Characterization of active metabolites from bio-guided fractionation of Thymus mastichina)
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 40 k€.

PTDC/QUI/65187/2006 Rational Design, Synthesis and Screening of an Indole Library for Novel Anti-Oxidant and Anti-Inflammatory Drug Candidates
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 151 k€.

PTDC/BIA-PRO/74498/2006 Characterization of a new family of heme-containing sensor proteins from Geobacter sulfurreducens
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 82 k€.

PTDC/QUI/70182/2006 Functional and structural characterization of PpcA: a key protein in metal reducing bacteria
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 126 k€.

PTDC/BIA-PRO/111141/2009 Protein-carbohydrate interaction characterization of Laforin – a human protein involved in lafora disease
BIOCANT - Associação de Transferência de Tecnologia (BIOCANT), Universidade do Minho (UM) and Centro de Neurociências e Biologia Celular (CNBC/UC)
Budget: 185.5 k€.

Bilateral Action FCT – ANR (Portugal/France) Agentes de Imagem Multimodal para detecção de placas A-beta amilóide na doença de Alzheimer
Centro de Neurociências e Biologia Celular (CNBC/UC)
Budget: 7 k€.

PTDC-SAU-MET-111398-2009 Role of the intestine in promoting the lipogenic effects of fructose
Centro de Neurociências e Biologia Celular (CNBC/UC), Department of Radiology - Radboud University Nijmegen Medical Centre (UMCN) and Universidade de Aveiro (UA)
Budget: 159.5 k€.

German Diabetes Foundation Endogenous glucose and glycogen metabolism in insulin resistant subjects
Centro de Neurociências e Biologia Celular (CNBC/UC)
Budget: 14 k€.

PTDC/SAU-FAR/118459/2010 Towards malaria eradication. A novel approach for multitargeting the parasite's life cycle
Faculdade de Farmácia da Universidade de Lisboa (FF/UL), Centro de Neurociências e Biologia Celular (CNBC/UC) and Instituto de Medicina Molecular (IMM/FM/UL)
Budget: 132 k€.

PTDC/QUI/QUI/122900/2010 Fibrils, Interrupted: Inhibiting Deviant Protein-Protein Interactions in Amyloids
Centro de Neurociências e Biologia Celular (CNBC/UC)
Budget: 114 k€.

Portuguese Cancer Charity Desenvolvimento de novos métodos auxiliares de diagnóstico e monitorização do cancro do pulmão com base nas assinaturas metabólicas detetadas por metabonómica
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA)
Budget: 5 k€.

PTDC/QUI/66523/2006 Estudo metabonómico de desordens da grávida e do feto por espectroscopia de Ressonância Magnética Nuclear (RMN): caracterização bioquímica e métodos de diagnóstico
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA) and Hospitais da Universidade de Coimbra, E.P.E (HUC/UC)
Budget: 76 k€.

PTDC/QUI/68017/2006 Caracterização metabólica e diferenciação bioquímica de tecidos tumorais de pulmão humano por métodos de Ressonância Magnética Nuclear (RMN)
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA) and Hospitais da Universidade de Coimbra, E.P.E (HUC/UC)
Budget: 71 k€.

PTDC/QUI/64203/2006 Estudos estruturais e funcionais de proteínas de ligação ao hemo da família SOUL/HBP
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA) and Fundação da Faculdade de Ciências e Tecnologia (FFCT/FCT/UNL)
Budget: 77.7 k€.

PTDC/QUI-QUI/100998/2008 Desenvolvimento de métodos de ressonância magnética nuclear de alta resolução para 1H e aplicações em materiais e moléculas de interesse biológico
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA)
Budget: 97 k€.

PTDC/QUI/65647/2008 New hydroxypyrimidinone-grafted solid chelating matrices for environmental and biological applications
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA)

ENERMATaa 2009-1/086, Funding Agency: Atlantic Area Transnational Cooperation Programme 2007-2013, Programme: (INTERREG IV B)

PTDC/MAR/100482/2008 Bioactive products in algae of Azores
Centro Interdisciplinar de Investigação Marinha e Ambiental (CIIMAR/CIMAR), Universidade de Aveiro (UA) and Universidade dos Açores (UAçores)
Budget: 148 k€.

PTDC/SAU-FAR/111414/2009 Developing strategies to understand antibiotics influx at a molecular level
Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares - Porto (ICETA-Porto/UP)
Budget: 160 k€.

PTDC/CTM/101484/2008 CHITOSAMP - CHITOSan-AntiMicrobial Peptide-based biomaterials for the treatment of osteomyelitis
Faculdade de Ciências da Universidade do Porto (FC/UP), Instituto de Biologia Molecular e Celular (IBMC/UP) and Instituto Nacional de Engenharia Biomédica (INEB Porto)
Budget: 185 k€.

PTDC/QUI-QUI/111060/2009 Novos compostos heterocíclicos anti-tumorais e anti-angiogénicos: Síntese, modelação molecular, screening de inibição enzimática e estudos em linhas celulares tumorais e endoteliais com receptores membranares de tirosina cinase como alvos
Universidade do Minho (UM), Instituto Politécnico de Bragança (IPBragança) and Faculdade de Medicina da Universidade do Porto (FM/UP)
Budget: 134.5 k€.

Ref. 04/12, CIMAGO (Centro de Investigação em Meio Ambiente, Genética e Oncobiologia – Medicine Faculty, Universidade de Coimbra) Estudo metabonómico do cancro do pulmão em estado cirúrgico: pesquisa de assinaturas metabólicas em tecidos e biofluidos
collaboration with Faculty of Medicine of the University of Coimbra, Hospitals of University of Coimbra
Budget: 1750 €.

Ref. 03/12, CIMAGO (Centro de Investigação em Meio Ambiente, Genética e Oncobiologia – Medicine Faculty, Universidade de Coimbra) Pesquisa de novos marcadores de resposta à terapêutica no cancro do pulmão
collaboration with Faculty of Medicine of the University of Coimbra, Hospitals of University of Coimbra
Budget: 1750 €.

Ref. Project between University of Aveiro/BP Amoco Chemical Company, November 2012 – November 2013: collaboration with BP Amoco Chemical Company Study of molecular sieve catalysts by analysis with NMR methods
Budget: 1750 €.

PTDC/QUI-QUI/117803/2010 ASTHMA: Future asthma management helped by non-evasive sampling: contributes for the definition of a rapid and non-evasive diagnostic tool
Universidade de Aveiro (UA), Fundacao da Faculdade de Ciencias – Universidade de Lisboa (FFC/FC/UL)
Budget: 90.5 k€.

PTDC/SAU-TOX/120953/2010 Metabolic profiling: a novel tool for evaluation of the toxicological and biological effects of nanomaterials
CICECO - Universidade de Aveiro (UA), Fundacao da Faculdade de Ciencias – Universidade de Lisboa (FFC/FC/UL)
Budget: 152.4 k€.

PTDC/QUI-BIQ/118389/2010 Structure-based design, biological activity and model membrane permeation studies of antimicrobial peptaibols bearing unnatural amino acids
Chemistry Center - Universidade do Minho (UM)
Budget: 99 k€.

PTDC/QUI-QUI/116864/2010 HEDICIN - HEterocycle-DIpeptide-CINnamic acid conjugates as novel antimalarials
Chemistry Research Center – Science Faculty, Universidade do Porto (FC/UP)
Budget: 68 k€.

Material Science

PTDC/FIS/110132/2009 New functional materials obtained from micro and nano cellulose fibers
Instituto Superior de Engenharia de Lisboa (ISEL/IPL) and Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa (FCT/UNL)
Budget: 148 k€.

PTDC/CTM/100244/2008 Development of Ion jelly thin film printable batteries for smart devices
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 175 k€.

PTDC/CTM/101538/2008 Optical Sensors and Nanomaterials for Anion Recognition
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA) and Instituto de Telecomunicações (IT)
Budget: 180 k€.

PTDC/QUI/65228/2006 Nanocages" e "bio"-polímeros para reconhecimento e solubilização de nanotubos de carbono
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA)
Budget: 122 k€.

PTDC/QUI/74150/2006 Síntese de Novos Materiais Multiporfirínicos
Unidade de Química Orgânica, Produtos Naturais e Agroalimentares (DQ/UA)
Budget: 72.5 k€.

PTDC/QUI-QUI/098098/2008 Redes Metalo-Orgânicas Nanométricas Baseadas em Polifosfonatos de Lantanídeos
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA)
Budget: 149 k€.

PTDC/QUI-QUI/105304/2008 Silica nanoparticles as supports for homogeneous catalysts: a gateway to Nanocatalysis
Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares - Porto (ICETA-Porto/UP)
Budget: 200 k€.

PTDC/CTM/108820/2008 Novel functional textiles obtained by incorporation of silica nanoparticles and carbon nanotubes: production, characterization and applications
Faculdade de Engenharia da Universidade do Porto (FE/UP), Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares - Porto (ICETA-Porto/UP) and CENTITVC - Centro de Nanotecnologia e Materiais Técnicos, Funcionais e Inteligentes (CENTI)
Budget: 170 k€.

PTDC/CTM-NAN/112428/2009 DENDRIMAT – New materials for drug/gene delivery based on the self-assembly of dendrimer-chitosan-single stranded DNA
Centro de Química da Madeira (CQM/UMA) and Instituto Nacional de Engenharia Biomédica (INEB Porto)
Budget: 151 k€

PTDC/CTM-NAN/1748/2012 DENDIMAGE – Development of Novel Dendrimer-Based Nanoparticles for Dual Mode Computed Tomography and Magnetic Resonance Imaging of Tumors
Centro de Química da Madeira (CQM/UMA)
Budget: 198 k€

PTDC/SAU-BEB/71161/2010 DENDRALGENE - Design of New Gene Delivery Vectors Based on Dendrimers, Alginate and the RGD Sequence for Bone Tissue Engineering
Centro de Química da Madeira (CQM/UMA)
Budget: 175 k€

SolSubC200801000088 -Project supported by the Regional Canary Island - Fabricación y estudio de

dispositivos híbridos orgánico-inorgánico para aplicaciones en optoelectrónica
Centro de Química da Madeira (CQM/UMA)
Budget: 35 k€

PTDC/CTM-NAN/116788/2010 Self-assembled nanoparticles based on PEG-PLA-dendrimer building blocks for dual gene/drug delivery
Centro de Química da Madeira (CQM/UMA)
Budget: 157 k€

PTDC/CTM/098451/2008 OPUSGRAFT - Oligo(phenylene ethynylene)s Derivatives Covalently Grafted Onto Porous Silicon: Novel Hybrid Molecular/semiconductor Systems for Application as Waveguides
Centro de Química da Madeira (CQM/UMA)
Budget: 168 k€

PTDC/QUI/64202/2006 FUNCMETAL - functionalized metallodendrimers based on 2,4,6-tri-substituted-1 ,3,5 - triazine derivatives dore
Centro de Química da Madeira (CQM/UMA)
Budget: 101 k€

PTDC/CTM/099595/2008 Stimuli-Responsive Cellulose Membranes built from Micro and Nano Helicoidal Fibers for Blood and Tissue Oxigenation
Faculdade de Ciencias e Tecnologia da Universidade Nova de Lisboa – FCT/UNL
Budget: 136 k€.

PTDC/QUI-QUI/117498/2010 Anchoring of metal nanoparticles on graphene hybrid assemblies with photoactive molecules
Instituto Superior Tecnico – Universidade Tecnica de Lisboa (IST/UTL) and Universidade de Aveiro (UA)
Budget: 101 k€.

PTDC/QUI-QUI/121857/2010 Development of conducting polymer based electrocatalysts for oxygen reduction in direct borohydride fuel cells
Fundacao da Faculdade de Ciencias – Universidade de Lisboa and Universidade de Aveiro (UA)
Budget: 114 k€.

Catalysis

PTDC/QUI-QUI/110080/2009 High Valent Oxo-complexes – A new class of Catalysts for C-X (X = C, N, O, S and P) Bond Forming Reactions
Instituto Superior Técnico (IST/UTL)
Budget: 85 k€.

PTDC/QUI-QUI/110532/2009 Carbohydrates as chiral scaffolds for the asymmetric synthesis of biologically important molecules
Instituto Superior Técnico (IST/UTL)
Budget: 80 k€.

PTDC/QUI-QUI/113910/2009 Mecanismos de bioactivação do fármaco anti-HIV Nevirapina: identificação de metabolitos reactivos e potencial mutagénico
Instituto Superior Técnico (IST/UTL), Faculdade de Farmácia da Universidade de Lisboa (FF/UL) and Faculdade de Ciências Médicas (FCM/UNL)
Budget: 133 k€.

PTDC/QUI-QUI/109846/2009 Chiral metalla-dianocarbene precatalysts for asymmetric catalytic reactions obtained by the metal-mediated approach
Instituto Superior Técnico (IST/UTL), Department of Chemistry, St. Petersburg State University (DC-SPSU) and Institute of Chemical Sciences and Engineering - Ecole polytechnique fédérale de Lausanne (ISIC-EFPL)
Budget: 63 k€.

PTDC/SAU-TOX/111663/2009 Toxicidade hepatica em indivíduos infectados pelo VIH expostos à nevirapina
Faculdade de Ciências Médicas (FCM/UNL), Instituto Superior Técnico (IST/UTL), Instituto de Tecnologia Química e Biológica (ITQB/UNL), Centro Hospitalar de Lisboa Central, EPE (CHLC), Hospital Amadora/Sintra - Sociedade Gestora, S.A. (HFF)
Budget: 131 k€.

PTDC/QUI-QUI/114139/2009 Inibição da Telomerase como alvo de novos complexos de Cu (II) anti-tumorais
Instituto Superior Técnico (IST/UTL) and Instituto Tecnológico e Nuclear (ITN)
Budget: 115 k€.

PTDC/QUI/69598/2006 Synthesis of Coumarin Derivatives with Potential Industrial Applications
Universidade de Evora (UE) and Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 96 k€.

PTDC/QUI/67933/2006 From Design to Synthesis of New Anti-Tubercular Agents.
Fundação da Faculdade de Ciências -FFC/FC/UL and Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 149 k€.

PTDC/QUI/66086/2006 Green production of cyclodextrin-based matrixes using supercritical carbon dioxide
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 99 k€.

PTDC/QUI/67786/2006 CHROMOGENICS: study and characterization of chromogenic materials
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 149 k€.

PTDC/QUI-QUI/104056/2008 The Development and Rationalization of Stereoselective Reactions in Some Chiral Systems. A mixed experimental and theoretical approach
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 140 k€.

PTDC/QUI-QUI/104129/2008 Catiões Flavílio Encapsulados
Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 66 k€.

PTDC/QUI-QUI/099388/2008 Unveiling the secrets of molecules with colour and history: from ancient to modern times
Universidade de Coimbra (UC) and Fundacao da Faculdade de Ciencias e Tecnologia – FFCT-FCT/UNL
Budget: 200 k€.
PTDC/QUI-QUI/112913/2009 Desenvolvimento de complexos metálicos suportados derivados do binaftilo. Sistemas multicatalíticos cooperativos para transformações assimétricas Tandem ortogonais
Centro de Química da Universidade de Coimbra (CQ/FCT/UC) and Instituto Superior Técnico (IST/UTL)
Budget: 138 k€.

PTDC/QUI-QUI/118078/2010 Fotoquímica de novas azidas: uma porta de entrada para o estudo de nitrenos
Centro de Química da Universidade de Coimbra (CQ/FCT/UC)
Budget: 129 k€.

PTDC/QUI-QUI/111879/2009 Controlo Óptico de Reacções Fotoquímicas Dependentes da Conformação Molecular
Centro de Química da Universidade de Coimbra (CQ/FCT/UC)
Budget: 150 k€.

PTDC/QUI-QUI/1103497/2009/ Sustainable catalysis based on N-heterocyclic carbene metal complexes (2011-2014)
Instituto de Tecnologia Química e Biológica (ITQB/UNL)

PTDC/QUI-QUI/113678/2009 Design of acid-functionalised periodic mesoporous organosilica catalysts for rections with/in water
Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (CICECO/UA), Fundação da Faculdade de Ciências (FFC/FC/UL) and Centre National de la Recherche Scientifique UMR6503 / Université de Poitiers (LACCO, UMR6503)
Budget: 135 k€.

PTDC/AGR-ALI/67579/2006 Novas Metodologias para o Estudo do Sabor de Alimentos: Interpretação do Fenómeno da Adstringência
Associação para o Desenvolvimento da Faculdade de Ciências (ADFC/FC/UP), Centro de Investigação em Química (CIQ/FC/UP) and Universidade de Aveiro (UA)
Budget: 100 k€.

Marie Curie Network; EU-ITN-215009 Natural Products and related Redox Catalysts: Basic Research and Applications in Medicine and Agriculture-(RedCat)

PTDC/QUI-QUI/102454/2008 Development of Organic Synthesis Methodologies Based on an Ohmic Heating Reactor
Unidade de Química Orgânica, Produtos Naturais e Agroalimentares da Universidade de Aveiro (DQ/UA), Universidade do Minho, Faculdade de Ciências - Universidade do Porto, e Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares – Porto – Universidade do Porto
Budget: 158 k€.

Annex 4

Supported MSc and PhD Thesis

STARTED IN 2010

Helena Cristina Gil Cardeira dos Santos Leitão PhD Project Title “Novos Biomarcadores em RM para a Esteatose, Inflamação e Fibrose Hepáticas”, Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).
Supervisor: Carlos F.G.C. Geraldes, Filipe Caseiro Alves
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/33893/2009)

Ana Marguerita Martins Metelo PhD Project Title “Development and Therapy Validation of Animal Models of Paediatric Medulloblastoma by Magnetic Resonance Methods”, Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).
Supervisor: M. Margarida Castro, Pilar Lopéz-Larrubia
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/70002/2010)

Vera Rute Pinto Augusto, PhD Project Title "Characterization of ionJelly® materials using different NMR techniques", Chemistry Department, Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2010).
Supervisor: Eurico Cabrita, Pedro Vidinha, Gabriel Feio
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/42322/2007)

Luisa Carvalho, PhD Project Title “Novel synthetic strategies towards glycosaminoglycans with anti-inflammatory activity”, Chemistry Department, Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2010).
Supervisor: Maria Manuel Marques, Eduarda Fernandes
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/63407/2009)

Ana Rita Bernardo Restani da Silva, PhD Project Title “Just in time Dendrimers”, Chemistry Department, Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2010).
Supervisor: Ana Aguiar-Ricardo, Vasco Bonifácio
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH / BD / 66858 /2009)

João Miguel Ribeiro Avó, PhD Project Title "Controlo fotoquímico da Reologia", Chemistry Department, Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2010).
Supervisor: Jorge Parola, João Carlos Lima
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH / BD /65127/2009)

Manuel Jardim, PhD Project “Octupolar Heterometallic dendrimers based on 2,4,6-tris-substituted-1,3,5-triazine core derivatives for NLO applications”, Madeira Chemistry Center – Universidade da Madeira (2010).
Supervisor: João Rodrigues
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/65036/2009)

Carla Francisco, PhD Project “Síntese e actividade antitumoral de compostos análogos do psoraleno”, Chemistry Department, Universidade do Minho (2010).
Supervisor: Lígia L. M. M. Rodrigues
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/48636/2008)

Vera Cristina Moreira Duarte, PhD Project “Síntese Enantiosselectiva de Imino-açúcares Através da Metodologia de Diels-Alder. Avaliação Biológica dos Produtos”, Chemistry Department, Universidade do Minho (2010).
Supervisor: António Gil Fortes
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/61290/2009)

Miguel Filipe Ferreira, PhD Project “Multifunctional Gold Nanoparticles for Magnetic Ressonance Imaging of tumours”, Chemistry Department, Universidade do Minho (2010).
Supervisor: José Alberto Martins
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/63994/2009)

André Fontes, PhD Project “Quelatos anfifílicos de Ga(III) e Gd(III) do tipo tetraaza para imagem médica mediada por receptores de péptidos”, Chemistry Department, Universidade do Minho (2010).
Supervisor: João Paulo André
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/63676/2009)

Arsénio Sá, PhD Project “Triazapolycarboxylate-based Ga(III) and Mn(II) chelates for medical imaging (PET,

gamma-scintigraphy and MRI)", Chemistry Department, Universidade do Minho (2010).
Supervisor: João Paulo André
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/63639/2009)

Mónica Lipinska PhD Project, Faculty of Sciences, Universidade do Porto (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/66297/2009)

João M.S. Cardoso, PhD Project Title "N-Heterocyclic carbenes as ligands for high oxidation state metal complexes and their use in oxidation processes", ITQB-UNL, Instituto de Tecnologia Química e Biológica (2010).

Ana Esteves, PhD Project Title "Unravelling the regulatory mechanisms in thermo-adaptation of hyperthermophilic archaea ", ITQB-UNL, Instituto de Tecnologia Química e Biológica (2010).

Joana Romão, MSc Thesis Title “Green” production of cyclodextrin-based matrixes using supercritical carbon dioxide, Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2010).

Yong Geng PhD Project Title, CENIMAT, Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/635574/2009)

Carla Maria Dias Marques de Oliveira, PhD Project Title “Oxidation Management of Alcoholic Beverages”, CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/64097/2009)

Cláudia M. M. Rocha, PhD Project Title " Investigation of the metabolic phenotype of lung cancer by Nuclear Magnetic Resonance (NMR) spectroscopy and Mass Spectrometry (MS) combined with multivariate statistics", CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/63430/2009)

Diana Isabel Soares Pereira Resende, PhD Project Title " Estudos de adições conjugadas 1,4 e 1,6 organocatalíticas na síntese assimétrica de compostos com interesse terapêutico", CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/62696/2009)

Inês Lamego, PhD Project Title "Suportes implantáveis para quimioterapia localizada do osteossarcoma", CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/63916/2009)

Leandro Miguel de Oliveira Lourenço, PhD Project Title "Nanocages” e “bio”-polímeros para reconhecimento molecular e solubilização de nanotubos de carbono", CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/64526/2009)

Mengistie Leweyehu, PhD Project Title "New sensor and actuator devices based on metal organic frameworks and Ln2O3 nanotubes/rods", CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/67108/2009)

Oualid Talhi, PhD Project Title "New synthetic routes and evaluation of the antioxidant and anti-inflammatory activity of novel xanthone and chromone derivatives", CICECO, Universidade de Aveiro (2010).
Financial Support: Marie Curie

Sandra Lopes da Silva, PhD Project Title "Aplicação da tecnologia RMN na caracterização de petróleos brutos e de correntes processuais de resíduos pesados", CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BDE/33879/2009)

Silvia Diaz, PhD Project Title "Metabonomics of urine and plasma for pregnancy monitoring and prediction of disorders of the mother, foetus and newborn", CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/64159/2009)

Susana Aveiro, PhD Project Title "Structural and functional studies of site-specific mutants of the p22 heme-binding/ transporting protein", CICECO, Universidade de Aveiro (2010).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/64519/2009)

STARTED IN 2011

Ana Rita Almeida, PhD Project Title “Síntese de ligandos bifuncionais quirais para o desenvolvimento de reacções multicomponente com catalisadores heterobimetálicos. Funcionalização de olefinas heteroaromáticas com potencial actividade biológica”, Chemistry Department, Faculty of Sciences and Technlogy, Universidade de Coimbra (2011).
Supervisor: Maria Miguéns Pereira
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/73190/2010)

Ana Godinho, PhD Project Title "Etravirine Risk Assessment: Synthesis and biological significance of DNA and protein adducts as toxicity biomarkers" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Alexandra Antunes and Matilde Marques
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/72301/2010)

Érica Fontes, PhD Project Title "Síntese e Fotoquímica de Cromóforos Orgânicos para Células Solares" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: M. Berberan-Santos
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/73999/2010)

Ivânia Cabrita, PhD Project "Hidratos de carbono como unidade estrutural quiral para a síntese assimétrica de moléculas biologicamente importantes" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Ana Cristina Fernandes
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/74280/2010)

Jaime Coelho, PhD Project "New synthetyc methodologies for the transformation of biomass derived intermediates to valuable molecules" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Carlos A. M. Afonso
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/73971/2010)

Miriam Sousa, PhD Project "Effect of artificial matrices into neural stem fate" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Frederico Castelo Ferreira
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/73560/2010)

Sowmiah Subbiah, PhD Project "New Ionic Liquids for Novel Applications" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Carlos A. M. Afonso, Luis Paulo Rebelo
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/74088/2010)

Natércia do Carmo Valente Teixeira, PhD Project "Síntese e purificação de prodelfinidinas: reatividade com antocianinas e estudo das suas propriedades físico-químicas e biológicas" Science Faculty – Universidade do Porto (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/70053/2010)

Alexandra Maria Neves Gaspar, PhD Project "New therapeutic approaches in cancer: Rational design and synthesis of new adenosine A3 receptor ligands" Science Faculty – Universidade do Porto (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/43531/2008)

Maria João Correia Pinto Carvalho de Matos, PhD Project "Síntese e avaliação farmacológica de compostos heterocíclicos de núcleo cumarínico: híbridos cumarina-resveratrol" Science Faculty – Universidade do Porto (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/61262/2009)

Elsa Margarida Barros dos Reis, PhD Project "Development of new adenosine receptor A3 ligands as a strategic approach for obtaining a drug candidate for anticancer therapy" Science Faculty – Universidade do Porto (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/79768/2011)

Nuno Tiago Barros Silva, PhD Project "Multi-Target Directed Drugs for Neurodegenerative Diseases" Science Faculty – Universidade do Porto (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/79671/2011)

José Carlos Santos Teixeira PhD Project "New mitochondria-targeted antioxidants based on cinnamic scaffold as a therapeutic solution for neurodegenerative diseases" Science Faculty – Universidade do Porto (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/79658/2011)

Cátia Isabel Canavezes Esteves, PhD Project "Recognition of biomedically relevant ions and molecules in physiological and non-physiological conditions: design, synthesis and evaluation of novel heterocycle-based systems and unnatural amino acids and short peptides as fluorimetric chemosensors", Chemistry Center of Universidade do Minho (2011).
Supervisor: Susana Paula Graça Costa, M. Manuela Marques Raposo Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/68360/2010)

Elina Margarida Ribeiro Marinho, PhD Project "Síntese de Heterociclos de azoto contendo o núcleo de piperazina como potenciais antipsicóticos", Chemistry Center of Universidade do Minho (2011).
Supervisor: M. Fernanda Proença
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/73659/2010)

Maria Helena Pereira Vilaça, PhD Project "Synthesis of new peptide derivatives that self-assemble into nanostructure hydrogels for biomedical applications" Chemistry Center of Universidade do Minho (2011).
Supervisor: Paula Margarida Ferreira, José Alberto Martins
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/72651/2010)

Nádia Rodrigues Senhorães, PhD Project "Síntese de derivados de purina como ligandos de recetores de adenosina" Chemistry Center of Universidade do Minho (2011).
Supervisor: Alice Maria Esteves
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/73721/2010)

Sandrina Alves Heleno, PhD Project "Metabolitos humanos importantes de compostos fenólicos resultantes da dieta com cogumelos silvestres comestíveis: síntese química e estudos das suas propriedades anti-oxidantes e anti-tumorais" Chemistry Center of Universidade do Minho (2011).
Supervisor: Maria João Queiroz, Isabel Cristina Ferreira (IPB), Anabela Rodrigues Martins (IPB)
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/70304/2010)

Cristiana Silva Faria, PhD Project Title "Development of cell factories for the efficient production of mannosylglycerate, a thermolyte with great potential in biotechnology" MIT Portugal Doctoral Programme, partner Institutions MIT, ITQB-UNL and Minho University (2011).

Dušica Radoš, PhD Project Title "Metabolic engineering of Corynebacterium glutamicum for the production of four-carbon polyols under biotransformation conditions" ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Débora Tavares, PhD Project Title "The nasopharyngeal ecosystem: studies on the nature of bacterial interspecies competition" ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Tiago Duarte, PhD Project Title "Towards improved production of complex biopharmaceuticals through systems biotechnology" ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Bruno Figueiredo PhD Project Title "Microporous Materials for Cs+ Sensing and Its Selective Removal from Aqueous Solutions", CICECO – Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/75457/2010)

Djenisa Helene Ascenção Rocha, PhD Project Title "A reactividade química como ferramenta no desenho de novos derivados de cromona e 4-quinolona com potencial aplicação biológica" CICECO – Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/68991/2010)

Joana Isabel Torrão da Costa, PhD Project Title "Materiais multiporfirínicos: síntese e estudos fotofísicos" CICECO – Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/75242/2010)

Joana Pinto, PhD Project Title "Análise metabonómica de plasma de mulheres grávidas para identificação de indicadores lipídicos de doenças da mãe e do feto" CICECO – Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/73343/2010)

Reda Ahmed, PhD Project Title "Post synthetic modification of metal organic frameworks" CICECO – Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/51269/2010)

David Miguel Gaspar Ferreira Dias, PhD Project Title "Biophysical studies of Multi-Protein Complexes interfaces in Fragment-based Drug Discovery" Life Sciences Department, Faculty of Sciences and Technlogy, Universidade Coimbra in collaboration with the Chemistry Department of Cambridge University (2011).
Supervisor: Carlos F.G.C.Geraldes; Co-supervisor: Dr. Alessio Ciulli Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/81735/2011).

Alexandre Filipe Guerreiro Borges, Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (FCT-UNL).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/61903/2009)

Felismina Teixeira Moreira, Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (FCT-UNL).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/66735/2009)

Ricardo Marçalo da Silva Marques, Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (FCT-UNL).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/74515/2010)

Carina Isabel Correia Crucho, Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (FCT-UNL).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/71648/2010)

Vanessa Correia, Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (FCT-UNL).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/74730/2010)

Margarida Coelho, Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (FCT-UNL).

Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/75094/2010)

Tiago Reis, Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (FCT-UNL).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/51188/2010)

STARTED IN 2012

Telma Silva, MSc Thesis Project Title "ORMOSIL nanoparticles: application to image potential by RM" Instituto Superior Tecnico, Lisbon Technical University (2012).

Inês S. L. Martins, PhD Project Title "Toxicity biomarkers from aromatic antiepileptic drugs (AEDs): Synthesis and assessment of covalent adducts with blood proteins" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2012).
Supervisor: A. A. Antunes, M. M. Marques
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/75426/2010)

Sabina Jaros, PhD Project Title "Design of Functional Metal-Organic Frameworks Driven by Cage-like Aminophosphine Building Blocks: New Materials for Advanced Applications" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2012).
Supervisor: Armando J.L. Pombeiro
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/77024/2011)

Marina Pires, PhD Project Title "A new methodology towards anti-inflammatory drugs: PEG-based synthesis and screening - a highly multidisciplinary approach" (FCT-UNL) Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa (2012).
Supervisor: Maria Manuel B. Marques
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/89518/2012)

Shrika G. Harjivan, PhD Project Title "Chemical modification of histones by NNRTI metabolites: a molecular basis for Non-AIDS Defining Cancers" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2012).
Supervisor: M. M. Marques
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/80690/2011)

Tetiana Anisimova, PhD Project Title "Efficient and straight-forward approach to the chiral metalla-aminocarbene precatalysts for asymmetric catalysis" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2012).
Supervisor: Armando J.L. Pombeiro
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/81459/2011)

Joana Carrola, PhD Project Title "Evaluation of the biological effects and toxicity mechanisms of silver nanoparticles through metabolic profiling of human cells" (CICECO/UA) Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/79494/2011)

Joana Lia Cardoso de Sousa, PhD Project Title "Desenvolvimento de novos métodos de síntese e avaliação da atividade antioxidante e anti-inflamatória de novos compostos polifenólicos" (CICECO/UA) Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/76407/2011)

João Manuel Marques Rodrigues, PhD Project Title "Síntese de sensores, funcionalização de nanopartículas e fibras ópticas para reconhecimento de Aniões" (CICECO/UA) Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/81014/2011)

Joana Filipa Gonçalves Pinto, PhD Project Title "Estudos sobre a aplicação do aquecimento óhmico à síntese orgânica" (CICECO/UA) Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/77807/2011)

Maria Cidália Rodrigues de Castro, PhD Project Title "Synthesis and characterization of donor-acceptor of pi-conjugated heterocyclic systems and transition metal complexes bearing heterocyclic moieties for nonlinear optical (NLO) applications" (CQ-UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Maria M. Raposo, António Maurício da Costa Fonseca
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/78037/2011)

Ana Maria Silva Soares, PhD Project Title "Photoactivable prodrugs based on oxygen and nitrogen heterocycles" (CQ-UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Maria do Sameiro Torres Gonçalves, Susana Paula Graça da Costa
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/80813/2011)

Cristina Rafaela dos Santos Albuquerque Guimarães, PhD Project Title "Toward antioxidant and antitumor properties of wild medicinal plants traditionally used in Portugal:

extracts, isolated flavonoids, and their human metabolites obtained by chemical synthesis" (CQ-UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Maria João Ribeiro Peixoto de Queiroz, Isabel Cristina Fernandes Rodrigues Ferreira, Ana Maria Pinto Carvalho
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/78307/2011)

Ana Isabel Gomes Peixoto Palha Rodrigues, MSc Thesis Project Title "Synthesis of new novobiocin derivatives as potential anticancer agents" (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Ana Alexandra Gomes Gonçalves, MSc Thesis Project Title "Synthesis of new chromene derivatives with potential anticancer activity" (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Ana Cláudia Ribeiro Leite, MSc Thesis Project "Optimization and in vitro e in vivo tests of compounds as anti-tubercular agents", (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Ana Isabel Ferreira Ribeiro, MSc Thesis Project "Synthesis and design of imidazole derivatives with potential", (CQ-UM) Chemistry Center – Universidade do Minho (2012).
Bruno Orlando Pinto da Cunha, MSc Thesis Project "Evaluation of the electrochemistry stability of fluorescent esters of amino acid", (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Carina Martins Carvalho, MSc Thesis Project "Peptides with antibiotic activity: synthesis, characterization and membrane permeabilization studies by fluorescence spectroscopy" (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Cláudia Regina Moreira Barroso, MSc Thesis Project "Complexes of Mn(II) for Magnetic resonance Imaging" (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Diogo Miguel Ferreira Sampaio, MSc Thesis Project "Synthesis of new purinones with potential antimicrobial activity" (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Marco Gabriel Morais da Cruz, MSc Thesis Project "Synthesis and antimicrobial activity of new nitrogen heterocycles" (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Joana Campos, MSc Thesis Project "Synthesis of new thienopyrimidine derivatives as potentials antitumorals and antiangiogenics with membranar receptors of tyrosine kinase as targets." (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Sílvia Daniela Alves da Cunha, MSc Thesis Project, "Synthesis of new and better oxiredutase xanthine inhibitors" (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Sofia Maria da Costa Pereira, MSc Thesis Project, "Synthesis of peptides containing resides of N-alkylated non proteinogenic amino acids", (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Vânia Isabel Baptista de Castro, MSc Thesis Project, "Solid phase synthesis assisted by MW of peptides containing unnaatural α,α-dialkylglicines", (CQ-UM) Chemistry Center – Universidade do Minho (2012).

Sara Pereira, MSc Thesis Project Title "Role of the intestine in promoting the lipogenic effects of fructose" (CICECO/UA) Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (2012).

Mónica Caseiro Fernandes, MSc Thesis Project Title "Síntese de calixpirróis e avaliação das suas propriedades como sensores cromogénicos" (CICECO/UA) Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (2012).

Nuno Mota, MSc Thesis Project Title "Fotodegradação do fármaco metoprolol em águas naturais e residuais" (CICECO/UA) Centro de Investigação em Materiais Cerâmicos e Compósitos – Universidade de Aveiro (2012).

Ana Catarina Pereira, MSc Thesis Project Title "Study of the morphogenic factor RodZ" ITQB-UNL, Instituto de Tecnologia Química e Biológica (2012).

Andre Manuel Ferreira Fonseca, PhD Project Title "Dual-Target Directed Drugs for Parkinson's Disease", Universidade do Porto (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/80831/2011)

Nuno Tiago Barros Silva, PhD Project Title "Multi-Target Directed Drugs for Neurodegenerative Diseases", Universidade do Porto (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/79671/2011)

José Carlos Santos Teixeira, PhD Project Title "New mitochondria-targeted antioxidants based on cinnamic scaffold as a therapeutic solution for neurodegenerative diseases", Universidade do Porto (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/79658/2011)

Bruno Miguel Macedo da Silva Reis, PhD Project Title "Aloe nano-engineered edible coatings", Universidade do Porto (2012).

Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/82414/2011)

Tânia Alexandra Fernandes de Sousa Moniz, PhD Project Title “Design of novel 3-hydroxy-4-pyridinone iron chelators to fight mycobacterium infection”, Universidade do Porto (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/79874/2011)

Carla Patrícia Queiroz, PhD Project Title “Síntese e caracterização de polímeros de coordenação multifuncionais: aplicação em catálise heterogénea e dispositivos óticos”, Universidade do Porto (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/79702/2011)

Ivo Emanuel Sampaio Dias, MSc Thesis Project Title “Síntese de Novos Tripéptidos Prolino-Miméticos Análogos dos Neuroprotetores PLG e GPE” Science Faculty – Universidade do Porto (2012).

Ana Sofia Martins Gomes, MSc Thesis Project Title “Síntese e avaliação de análogos da cloroquina e da quinacrina como novos protótipos antimaláricos” Science Faculty – Universidade do Porto (2012).

Marta Maia, MSc Thesis Project Title “MAO-B Directed Drugs for Parkinson Disease” Science Faculty – Universidade do Porto (2012).

Lisa Sequeira, MSc Thesis Project Title “Design and synthesis of novel antioxidants based on natural scaffolds” Science Faculty – Universidade do Porto (2012).

Ricardo Amorim, MSc Thesis Project Title “Design and synthesis of novel mitochondriotopic antioxidants” Science Faculty – Universidade do Porto (2012).

CONCLUDED IN 2010

Neuza Luisa da Silva Domingues, MSc Thesis “VO(dmpp)2 um composto com promissoras propriedades anti-diabeticas – seu modo de administração, transporte e captação e estudo da sua acção a nível da cascata de sinalização da insulina” Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).

Catia Melo, MSc Thesis “VO(dmpp)2 um composto com promissoras propriedades anti-diabeticas – Estudo da sua acção no metabolismo de glucose e lipidos nos vários orgaos e tecidos” Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).

Andreia Raquel Esteves de Sousa, MSc Thesis “Estudos RMN e de luminescência da complexação dos iões Al3+ e Ga3+ com hidroxisulfoquinolina” Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).

Joana Simões, MSc Thesis “Sondas luminescentes baseadas em bases de Schiff para a detecção de metais pesados“” Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).

Ana Marguerita Martins Metelo MSc Thesis “A new Vanadium Compound as a promising insulin-mimetic drug: Ex vivo and in vivo studies to clarify its mechanism of pharmacological action”, Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).

Joana Sofia Rodrigues Barra, MSc Thesis “Metabolic Profiling of Cardiac Cachexia in an Animal Model” Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).

Ana Rita Simões Gonçalves, MSc Thesis “Quantifying de novo lipogenesis in animal models by 2H2O and 2H NMR” Department of Life Sciences, Faculty of Sciences and Technlogy, Universidade de Coimbra (2010).

Sandra Isabel Pereira Dias, MSc Thesis “Estudo de efeito de memoria em dispositivos PDLC” CENIMAT, Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2010).

Catarina Sofia Romão Charneira, MSc Thesis "Avaliação da toxicidade do fármaco anti-HIV abacavir: síntese e caracterização estrutural de possíveis biomarcadores", Chemistry Department, Universidade Nova de Lisboa (2010).

Luís Carlos da Cruz Magalhães, MSc Thesis "Pilot study of structural proteomics thermostable proteins from sulphurisphaera SP. By NMR", Chemistry Department, Universidade Nova de Lisboa (2010).

Carina Isabel Correia Crucho, , MSc Thesis “Complexos de ferro quirais para oxidações estereosselectivas de hidrocarbonetos", Chemistry Department, Universidade Nova de Lisboa (2010).

Anna Vadymivna Kladova, PhD Thesis "Metals in proteins from sulphate-reducing bacteria: adenylate kinase and ATP sulfurylase", Chemistry Department, Faculty of Sciences and Technology, Universidade Nova de Lisboa (2010).

Pedro Manuel da Cunha Catalão Pires dos Santos, PhD Thesis “Mecanismos de degradação de compostos de relevância biológica por radicais oxidantes”, Chemistry Department, Faculty of Sciences and Technology, Universidade Nova de Lisboa (2010).

Rui Miguel Lourenço Rocha de Almeida, MSc Thesis "NMR Studies of transient protein complexes", Chemistry Department, Faculty of Sciences and Technology, Universidade Nova de Lisboa (2010).

André Alexandre Cotta Guerra Vidal Pinheiro, MSc Thesis "Light controlled synthesis of nucleic acids", Chemistry Department, Faculty of Sciences and Technology, Universidade Nova de Lisboa (2010).

Riccardo Wanke, PhD Thesis “Nitrogen and oxygen-based chelating ligands: tris(pyrazolyl)methane and salicylaminedate ligands”, (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2010).

Sonia Duarte Barroso, PhD Thesis “Early Transition Metal Diamine-Bisphenolate Complexes: Synthesis, Structures and Applications”, (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2010).

Ana Paula Gonçalves Batista, PhD Thesis "Energy transduction by respiratory complex I", ITQB-UNL, Instituto de Tecnologia Química e Biológica (2010).

Catarina Sofia Romão Charneira, MSc Thesis "Avaliação da toxicidade do fármaco anti-HIV abacavir: síntese e caracterização estrutural de possíveis biomarcadores” (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2010).

Inês Sofia Lança Martins, MSc Thesis "Síntese e avaliação citotóxica de compostos orgânicos contendo o grupo funcional seleno-carbonilo" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2010).

David Miguel Alves Novais, MSc Thesis "Oxidação Química e enzimática de 2-hidroxinevirapina" (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2010).

Elena Valishina, MSc Thesis “Novel highly-efficient palladium-aminocarbene precatalysts for cross-coupling reactions under mild conditions” (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2010).

Alexander Tskhovrebov, MSc Thesis “Metal-mediated dipolar cycloaddition of nitrones to metal-bound isonitriles”, (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2010).

André Melão Alcantâra, MSc Thesis “Análise da variação da Trealose-6-fosfato em Medicago truncatula sujeita a deficit hídrico”, ITQB-UNL, Instituto de Tecnologia Química e Biológica (2010).

Ewa Krol, MSc Thesis “Production and isolation of Cholera Toxin B-Subunit for future NMR experiments with plant extracts” ITQB-UNL, Instituto de Tecnologia Química e Biológica (2010).

Catarina Alexandra Veríssimo Esteves, MSc Thesis "Desenvolvimento de quelantes macrocíclicos para complexação de iões metálicos de transição e lantanídeos com interesse em aplicações médicas", ITQB-UNL, Instituto de Tecnologia Química e Biológica (2010).

Cristiana Silva Faria, MSc Thesis “Engineering Saccharomyces cerevisiae for the production of mannosylglycerate - a yeast model for assessing its application in protein stabilization”, ITQB-UNL, Instituto de Tecnologia Química e Biológica (2010).

Luís Carlos Magalhães, MSc Thesis “Pilot study of structural proteomics thermostable proteins from Sulphurisphaera sp. by NMR”, ITQB-UNL, Instituto de Tecnologia Química e Biológica (2010).

Patrícia Figueiredo, MSc Thesis “Alterações no metaboloma e no metabolismo do carbono de amostras biológicas expostas a stress", CICECO, Universidade de Aveiro (2010).

Juliana Crespo, MSc Thesis “Alterações no metaboloma de osteoblastos por exposição a nanopartículas (NPs) de Fe3O4,Au desenvolvidas para entrega selectiva de fármacos", CICECO, Universidade de Aveiro (2010).

Andreia Gerniski Macedo, PhD Thesis “Nanotubos e nanobastonetes de óxidos de latanídeos: síntese, processamento, luminescência e propriedades catalíticas”, CICECO, Universidade de Aveiro (2010).

Andreia Sofia Filipe Farinha, PhD Thesis “Calix[4]pirróis – síntese e aplicação como sensores de aniões”, CICECO, Universidade de Aveiro (2010).

Cláudia Marisa Barreiros Neves, MSc Thesis “Oxidação biomimética de fármacos", CICECO, Universidade de Aveiro (2010).

Joana Isabel Torrão da Costa, MSc Thesis “Síntese de sistemas multiporfirínico via reacções de "click"”, CICECO, Universidade de Aveiro (2010).

Joana Pinto, MSc Thesis “Análise metabonómica de plasma de mulheres grávidas para identificação de indicadores lipídicos de doenças da mãe e do feto”, CICECO, Universidade de Aveiro (2010).

João Manuel Marques Rodrigues, MSc Thesis “Sistemas supramoleculares baseados em porfirinas: síntese e propriedades”, CICECO, Universidade de Aveiro (2010).

Patrícia Alexandra Amaro Martins Vaz, MSc Thesis “Estudos de síntese e transformação de novos derivados de quinolonas”, CICECO, Universidade de Aveiro (2010).

Sara Mirassol Tomé, MSc Thesis "(E)-C-Glicosil-2-estirilcromonas com potencial actividade antioxidante", CICECO, Universidade de Aveiro (2010).

Maria João Menezes de Carvalho, MSc Thesis "Isolamento e caracterização de princípios activos da Madre de Louro e de Lauraceas da Madeira", Madeira Chemistry Center – Universidade da Madeira (2010).

Neide Freitas, MSc Thesis "Encapsulation of Single hMSCs in Polyelectrolyte shells - Preliminary Studies", Madeira Chemistry Center – Universidade da Madeira (2010).

Ana Maria Silva Soares, MSc Thesis "Bioconjugados fluorescentes: síntese e aplicação em estudos de clivagem foto-induzidos", Chemistry Center, Universidade do Minho (2010).

Natália Sofia Dias, MSc Thesis "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", Chemistry Center, Universidade do Minho (2010).

João Carlos Gonçalves, MSc Thesis "Síntese de carbolinas com potencial actividade biológica", Chemistry Center, Universidade do Minho (2010).

Nádia Rodrigues Senhorães, MSc Thesis "Síntese de novos ligandos para receptores de Adenosina", Chemistry Center, Universidade do Minho (2010).

Ana Luísa, MSc Thesis "Marcadores fluorescentes de biomoléculas: Síntese e propriedades fotofísicas", Chemistry Center, Universidade do Minho (2010).

Maria Helena Pereira Vilaça, MSc Thesis "Síntese de derivados Cíclicos de RGD", Chemistry Center, Universidade do Minho (2010).

Manuel Ricardo da Costa Calhelha, PhD Thesis "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", Chemistry Department, Universidade do Minho (2010).
Supervisor: Maria-João R.P. Queiroz
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/29274/2006)

Luís Miguel Neves Ferreira Serra Cruz, PhD Thesis "Estudo dedas reacções entre catequinas e antocianinas. Síntese de novos compostos", Science Faculty of Universidade do Porto (2010).

CONCLUDED IN 2011

Ana Francisca Leal Silva Soares, PhD Thesis "Profiling the control of hepatic glucose and lipid metabolism for evaluating novel strategies of insulin delivery", Life Sciences Department, Faculty of Sciences and Technlogy, Coimbra University (2011).

Sónia Luzia Claro de Pinho, PhD Thesis "Nanopartículas Multifuncionais para Imagem de RM e Fluorescência", Faculty of Sciences and Technlogy, Universidade de Coimbra in collaboration with CICECO – Universidade de Aveiro (2011).

João Henrique Pires de Almeida Alexandre, PhD Thesis "Sistemas Elastoméricos de Rede Aleatória: Preparação e caracterização molecular, estrutural e dinâmica, dos reticulados. Correlação com as propriedades macroscópicas" at CENIMAT/I3N, Faculty of Sciences and Technlogy – Universidade Nova de Lisboa (2011).

João Jorge, MSc Thesis "Bioengineering of Lactococcus lactis through modulation of its major glucose transporter", ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).
Supervisor: Ana Rute Neves

Marta Viseu Rodrigues, PhD Thesis "Heat Stress Adaptation in Hyperthermophiles: Biosynthesis of Inositol-Containing Compatible Solutes", ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Tiago Vasconcelos Duarte Moreira Pais, PhD Thesis "Insights into the Molecular Mechanisms of Protein Stabilization by Osmolytes of Hyperthermophiles" ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Ana Isabel Porém Amaral PhD Thesis "Metabolic Flux Analysis of neural cell metabolism in primary cultures" ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Pedro Miguel Veríssimo Mateus PhD Thesis "Ditopic molecular architectures for the recognition of anionic species" ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Ana Raquel Macedo Soares, PhD Thesis "Phthalocyanine-based systems: synthesis, properties and applications", Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/29362/2006)

Ana Teresa Peixoto de Campos Gomes, PhD Thesis "Novos derivados porfirínicos: Síntese e potenciais aplicações em PDT", Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/38527/2007)

Carla M. B. Carvalho, PhD Thesis “Síntese e reactividade de benzo- e pirroloporfirinas”, Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/38611/2007)

João Aleixo Rodrigues, PhD Thesis “Desenvolvimento de métodos de Espectroscopia de Ressonância Magnética Nuclear (RMN) para o controlo da qualidade da cerveja e seu processo de fabrico”, Universidade de Aveiro (2011).

Mariana Fernandes, PhD Thesis ''Multi functional organic-inorganic hybrids prepared through sol-gel and/or self-assembly'', Universidade de Trás-os-Montes e Alto Douro in collaboration with Universidade de Aveiro (2011).

Raquel S. G. R. Seixas, PhD Thesis “Novos métodos de síntese de 4-quinolonas e benzo[b]acridonas”, Universidade de Aveiro (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/30734/2006)

Sónia Pinho, PhD Thesis “Multifunction Nanoparticles for MR and Fluorescence Imaging”, Universidade de Aveiro, Universidade de Coimbra, Universite Bordeaux I, Institut de Chimie de la Matiere Condensee de Bordeaux (2011).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/38313/2007)

Vanda I. R. Canelas, PhD Thesis “Síntese e potencialidades de aplicação de novos derivados porfirínicos”, Universidade de Aveiro (2011).

Sandra Cristina Gonçalves Gouveia, PhD Thesis “Phytochemical studies of bioactive Asteraceae plants endemic from Madeira Archipelago”, Madeira Chemistry Center – Universidade da Madeira (2011).
Supervisor: Paula Castilho
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/24227/2005)

Andreia Peixoto, PhD Thesis “Desenvolvimento de Novos Catalisadores de Metais de Transição. Catálise de Reacções de Carbonilação Conducentes à Obtenção de Produtos de Valor Acrescentado”, Chemistry Department, Universidade de Coimbra (2011).

Ana Sofia Ferreira, PhD Thesis “Activação de alcinos por complexos de Pd (II) ou Pt (II) com ligandos derivados da Cânfora”, (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Fernanda Carvalho
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/30339/2006)

Artur B. Lourenço, PhD Thesis “Yeast responses and determinants of resistance to propionic acid or ethanol at a systems level: chemogenomic and metabolomic strategies”, (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Isabel Sa-Correia
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (ABL/SFRH/BD/23437/2005)

Pedro Adao, PhD Thesis “Chiral Transition Metal Complexes as Catalysts for Sustainable Oxygen Transfer Reactions” (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: João Costa Pessoa
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRD/BD/40279/2007)

Pedro Morgado, PhD Thesis “Semifluorinated Alkanes - Structure-Properties Relations” (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Eduardo J. M. Filipe
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/39150/2007)

Ricardo José da Rocha Fernandes, PhD Thesis “Bioinspired Iron and Copper Catalyzed Oxidations and Reactions in Supercritical CO2” (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2011).
Supervisor: Armando J. L. Pombeiro
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/31150/2006)

Simone Dell’Acqua, PhD Thesis “Characterization of the activity of Nitrous Oxide Reductase: Biochemical, Spectroscopic and Mimetic Approaches” (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Filipa Alexandra Delgado Siopa, PhD Thesis “Modificação de proteínas e DNA por quinonas derivadas de catecolaminas”, (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Mara Lilia Soares da Silva, PhD Thesis “Development of molecularly imprinted polymers using supercritical fluid technology”, (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Bruno André Cunha de Vallêra Jacques Pedras, PhD Thesis “Synthesis, characterization and applications of new schiff base fluorescent chemosensors for metal and DNA interactions: conventional and “green” approaches” (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Alexandra Emanuela R. Ribeiro, PhD Thesis “Síntese de Imidazoles substituídos e N-óxidos heterocíclicos com potencial atividade antioxidante” Chemistry Center of Universidade do Minho (2011).
Supervisor: M. Alice Carvalho

Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/24760/2005)

Marta Sílvia Freitas da Costa, PhD Thesis “Síntese de novos compostos para “screening” como agentes antipsicóticos” Chemistry Center of Universidade do Minho (2011).
Supervisor: M. Fernanda Proença
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/31531/2006)

Rosa Maria Ferreira Batista, PhD Thesis “Síntese e caraterização de compostos heterocíclicos e de aminoácidos modificados com aplicação em óptica não-linear e/ou como sensores fluorimétricos e colorimétricos de aniões e catiões” Chemistry Center of Universidade do Minho (2011).
Supervisor: M. Manuela Raposo, Susana Paula Costa
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/36396/2007)

Andreia Daniela Moreira da Cruz Leite, PhD Thesis “Design de ligandos quelantes multifuncionalizados derivados de 3,4-hidroxi-piridinonas”, Science Faculty – Universidade do Porto (2011).

Rui Miguel Freitas Gonçalves, PhD Thesis “Interação entre compostos fenólicos e enzimas digestivas: relação estrutura-função”, Science Faculty – Universidade do Porto (2011).

Carlos Alberto Duarte Sousa PhD Thesis “Estudo e aplicação de reacções de cicloadição entre ciclopentadieno e oximas na síntese de análogos pirrolidínicos N-fosforilados”, Science Faculty – Universidade do Porto (2011).

Ivone Margarida Nunes Ferreira Vieira Peres, PhD Thesis “Nanoencapsulation of Active Compounds” Science Faculty – Universidade do Porto (2011).

Saúl Silva, MSc Thesis “Synthesis and reactions of 2-Oxoazabicyclo-[X.1.0]-alkanes” ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Vanessa Miranda, MSc Thesis “Tartaric Acid as starting material for the synthesis of chiral molecules” ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Catarina Alexandra Veríssimo Esteves, MSc Thesis "Desenvolvimento de quelantes macrocíclicos para complexação de iões metálicos de transição e lantanídeos com interesse em aplicações médicas", ITQB-UNL, Instituto de Tecnologia Química e Biológica (2011).

Hélia Filipa Baião Jeremias, MSc Thesis “Cytotoxic oxysteroids: synthesis and biological evaluation”, Pharmacy Faculty, Universidade de Coimbra.

Guido Rocha Lopes, MSc Thesis “Cromonas: estudos de biotransformação em derivados de valor acrescentado” CICECO – Universidade de Aveiro (2011).

Liliana Neto Costa, MSc Thesis “Fosfatos e Fosfonatos metálicos: Nova geração de catalisadores em síntese orgânica” CICECO – Universidade de Aveiro (2011).

Marta Pinheiro, MSc Thesis “Alterações no metaboloma de células humanas de fígado por exposição ao polissacarídeo carragenano como veículo de entrega de fármacos” CICECO – Universidade de Aveiro (2011).

Pedro António Martins Mira Varandas, MSc Thesis “Síntese enantiosseletiva de 1,2-di-hidropiridinas” CICECO – Universidade de Aveiro (2011).

Stéphanie Branco Leal, MSc Thesis “Síntese e transformação de 3-cinamoílcromonas” CICECO – Universidade de Aveiro (2011).

Tiago André Gomes Duarte, MSc Thesis “Estudos catalíticos na presença de polioxometalatos em fase homogénea e heterogénea” CICECO – Universidade de Aveiro (2011).

Ana Filipa Ladeirinha, MSc Thesis “Establishment of primary cell cultures from lung tissue biopsies and study of the cellular metabolic responses to cisplatin and radiation exposure”, CICECO, Universidade de Aveiro and Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Andreia F. F. Silva, MSc Thesis “Nitronas: Estudos de síntese e reactividade”, CICECO, Universidade de Aveiro (2011).

Dora C. S. Costa, MSc Thesis “Síntese e avaliação biológica de novos derivados porfirínicos”, CICECO, Universidade de Aveiro (2011).

Frederico R. Baptista, MSc Thesis "Síntese de (E)-2-Estirilcromonas C-preniladas", CICECO, Universidade de Aveiro (2011).

Gabriela N. Santos, MSc Thesis “Relatório de estágio em assuntos regulamentares – Grupo Tecnimede”, CICECO, Universidade de Aveiro (2011).

Patrícia Figueiredo, MSc Thesis “Efeitos de agentes de stress ambiental sobre o metaboloma da alface”, CICECO, Universidade de Aveiro (2011).

Sandra E. M. F. Marques, MSc Thesis “Simulações computacionais no ensino do equilíbrio químico” CICECO, Universidade de Aveiro (2011).

Teresa A. F. Cardote, MSc Thesis “Síntese de derivados corrólicos com actividade antimicrobiana” CICECO, Universidade de Aveiro (2011).

Vânia Patrícia Castro Teixeira Freitas, MSc Thesis “Materiais Híbridos Orgânicos-Inorgânicos Nanoestruturados para Aplicação em Fotónica”, CICECO, Universidade de Aveiro in collaboration with Universidade do Minho (2011).

Joana Margarida Franco Dantas, MSc Thesis “Follow the red road of tri-heme cytochromes in Geobacter sulfurreducens”, (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Ana Paula Fernandes, MSc Thesis “Characterization of a multiheme protein functioning as bacterial electronic capacitor” (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

João Luz, MSc Thesis “Bionanossondas de Citocromo e Nanopartículasde Ouro para Biorremediação de Crómio (VI)” (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Rute Isabel dos Santos Carvalho, MSc Thesis “Uma abordagem a sistemas de crescimento celular apical: síntese de um sensor para iões citosólicos de potássio” (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Patrique Nelson Ramos Nunes, MSc Thesis “Dynamic and interaction of cytochrome c with Pf1 virus” (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Ana Fiipa Correia Gomes, MSc Thesis "Pesquisa de substâncias ilícitas em suplementos alimentares" (FCT-UNL), Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Joana Isabel Sobral Romão, MSc Thesis “Development of cyclodextrin –hydrogel polymeric systems in scCO2 for drug delivery” Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

Cátia João Borges Silva, MSc Thesis “Efeito da velocidade de polimerização na eficiência de PDLCs” Chemistry Department of Faculty of Sciences and Technlogy, Universidade Nova de Lisboa (2011).

David Miguel Gaspar Ferreira Dias, MSc Thesis “High-Resolution Saturation Transfer Difference (STD) 1H NMR techniques and Docking simulations applied to Protein-ligand interactions” Faculty of Sciences and Technlogy, Universidade de Coimbra (2011).

Henrique Daniel F. Carvalho, MSc Thesis “Structural, Physicochemical and Photophysical Studies of New Cyclen Derivatives and Evaluation of Their Potential as MRI and MRI/NIR Probes” Faculty of Sciences and Technlogy, Universidade de Coimbra (2011).

Rui Filipe Silva Carvalho, MSc Thesis “Nanopartículas como potencias agentes de contraste para Imagem de Ressonância Magnética: caracterização físico-química de polioxometalatos (POMs) contendo iões lantanídeos (III) e suas nanopartículas revestidas de sílica” Faculty of Sciences and Technlogy, Universidade de Coimbra (2011).

Filipa Carvalho, MSc Thesis “Noninvasive analysis of hepatic acetyl-CoA by Chemical Biopsy” Faculty of Sciences and Technlogy, Universidade de Coimbra (2011).

Andreia Raquel Esteves de Sousa, MSc Thesis “Estudo da complexação da 8-hidroxi-5-sulfoxiquinolina com os metais alumínio e gálio em solução aquosa”, Faculty of Sciences and Technlogy, Universidade de Coimbra (2011).

Joana Filipa Costa Simões, MSc Thesis “Estudo de bases de Schiff para a complexação e detecção de metais pesados”, Faculty of Sciences and Technlogy, Universidade de Coimbra (2011).

Marisol Gouveia, MSc Thesis “Preparation of Low-generation metallodendrimers using nitrile-functionalized poly(alkylidenamines) dendrimers: cytotoxicity studies in cancer cell lines” Chemistry Department – Universidade da Madeira (2011).

Carla Miguel, MSc Thesis “Multilayered Core/Shell Nanoparticles of FeOX/Au/Ag” Chemistry Department – Universidade da Madeira (2011).

Cláudia Camacho, MSc Thesis “Polímeros condutores em monocamadas automontadas para a determinação de compostos de interesse ambiental” Chemistry Department – Universidade da Madeira (2011).

Daniel Bezerra de Lima, MSc Thesis “Coating of Implant Biomaterials Through the Layer-by-Layer Technique” Chemistry Department – Universidade da Madeira (2011).

Rita Castro, MSc Thesis “New Dendrimer-based Vectors for Antisense Therapy” Chemistry Department – Universidade da Madeira (2011).

Joana Mendes, MSc Thesis “Síntese de hidrogeis de base acrílica recorrendo a técnicas de polimerização radicalar viva. Potencial aplicação como fármacos poliméricos”, Chemical Engineering Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Catarina Inês Sanches Pinto, MSc Thesis "AZT-Molécula de Morte e Sobrevivência Celular", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Patrícia Isabel Miranda de Jesus, MSc Thesis "Avaliação Morfológica e Molecular na Administração Experimental de 7,12-Dimetilbenzantraceno", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

César Augusto Silva Henriques, MSc Thesis "Síntese de meso-porfirinas mistas – Estudos fotofísicos e térmicos", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Ângela Cristina Barrôco Neves, MSc Thesis "Caracterização estrutural pelo método semi-empírico, PM6, de complexos de ródio modificados com ligandos de piridina-difosfitos derivados do Bis-NAFTOL", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Juvêncio de Castro Ruas MSc Thesis "Extracção e caracterização do óleo das sementes da planta Champalo (Calophyllum inophyllum). Estudo de transesterificação catalítico para preparação de biodiesel", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Filipe André Gomes dos Reis Pimentel, MSc Thesis "Síntese de Ligandos Quirais para Alquilação Enantiosselectiva de Aldeídos e Reacção de Strecker Assimétrica", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Mariana Cavaca Marcos, MSc Thesis "Determinação de Medicamentos Antiepilépticos e Anticonvulsivantes por UPLC-MS/MS", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Marina Pires MSc Thesis "Síntese de Precursores de Radiofármacos para Detecção de Hipóxia Tumoral", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Célia Catarina Teixeira Frias Ferreira, MSc Thesis "Caracterização por GC-MS de glícidos. Derivatização assistida por microondas", Chemistry Department, Faculty of Sciences and Technology, Universidade de Coimbra (2011).

Alexandra M. Fernandes Brito, MSc Thesis "Síntese e Reatividade de N-Óxidos de pirimidina para síntese de novas moléculas com potencial atividade biológica", Chemistry Center of Universidade do Minho (2011).

António Manuel Pereira Ribeiro, MSc Thesis "Síntese de quinolinas com potencial antipalúdico", Chemistry Center of Universidade do Minho (2011).

Davide Ribeiro da Cruz, MSc Thesis "Desenvolvimento e validação de metodologias computacionais de desenho de fármacos baseado em fragmentos químicos", Chemistry Center of Universidade do Minho (2011).

Gonçalo Manuel Alves Ribeiro, MSc Thesis "Modifification of tumor-seeking peptides with fluorescent and metalchelating non-proteinogenic amino acids bearing heterocyclic", Chemistry Center of Universidade do Minho (2011).

Hugo Ricardo Matos Viana, MSc Thesis "Síntese de derivados de tienopiridinas como potenciais compostos anti-tumorais e/ou antiangénicos" Chemistry Center of Universidade do Minho (2011).

Carla Maria Cunha Mendes Lopes, MSc Thesis "Síntese de imidazolidinonas", Chemistry Center of Universidade do Minho (2011).

Luís Miguel dos Santos Conde, MSc Thesis "Polímeros naturais para aplicações biomédicas", Chemistry Center of Universidade do Minho (2011).

Daniela Peixoto, MSc Thesis "Síntese de novos derivados de tienopiridinas como potenciais compostos anti-tumorais e/ou antiangiogénicos", Chemistry Center of Universidade do Minho (2011).

Ana Daniela Gonçalves Firmino, MSc Thesis "Síntese e propriedades fotofísicas de novos derivados fluorescentes de (benzo)fenoxazina" Chemistry Center of Universidade do Minho (2011).

Ana Suarez, MSc Thesis "Synthesis of non-natural amino acids and peptides" Chemistry Center of Universidade do Minho (2011).

Ashly Tania da Cruz Rocha, MSc Thesis "Síntese de novos derivados de purina para estudos SAR no Micobacterium tuberculosis" Chemistry Center of Universidade do Minho (2011).

Rosa Cristina Moutinho Ferreira, MSc Thesis "Síntese de benzoxazolil-alaninas funcionalizadas com heterociclos de enxofre e oxigénio e estudos de interacção com catiões metálicos com importância biomédica" Chemistry Center of Universidade do Minho (2011).

Cristina Elisabete Araujo Sousa, MSc Thesis "Síntese de derivados da 1-Deoximanojirimicina" Chemistry Center of Universidade do Minho (2011).

Daniela Salgueiro, MSc Thesis "Estudos de diastereoselectividade de diversos dienófilos com dienos

derivados da D-Eritrose com vista à síntese de aza-açúcares e outros compostos" Chemistry Center of Universidade do Minho (2011).

Rui Daniel Vilaça Fernandes, MSc Thesis "Péptidos com actividade antibiótica: sintese de miméticos e estudos de permeabilização de membrana por espectroscopia de fluorescência" Chemistry Center of Universidade do Minho (2011).

Nádia Romeu Aguiam, MSc Thesis "Síntese de derivados de aminoácidos α, α-dissubstituídos e de péptidos contendo estes aminoácidos por reação de Ugi em fase sólida" Chemistry Center of Universidade do Minho (2011).

Patrícia Manuela Ribeiro Batista, MSc Thesis "Síntese e avaliação de novos aminoácidos funcionalizados com unidades de éter de coroa e benzoxazole como sensores fluorimétricos de catiões" Chemistry Center of Universidade do Minho (2011).

Marlene Andreia Pereira Costa, MSc Thesis "Síntese e determinação quantitativa da distribuição de antioxidantes em emulsões óleo/água e correlação com a sua capacidade antioxidante" CEMUP – Universidade do Porto (2011).

Ester Sofia Benfeito, MSc Thesis "Desenvolvimento de novos antioxidantes baseados no ácido cinâmico" CEMUP – Universidade do Porto (2011).

Jose Dias, MSc Thesis "Encapsulação de compostos bioactivos" CEMUP – Universidade do Porto (2011).

Ana Catarina Oliveira, MSc Thesis "Desenvolvimento de novos antioxidantes baseados no ácido benzoico" CEMUP – Universidade do Porto (2011).

Ana Amorim, MSc Thesis "Design de novos fluoróforos utilizando novas metodologias mais limpas e mais eficientes" CEMUP – Universidade do Porto (2011).

Tânia Alexandra Fernandes de Sousa Moniz, MSc Thesis "Novas arquiteturas moleculares para combater processos infeciosos", Science Faculty – Universidade do Porto (2011).

Inês Cardoso, MSc Thesis "Síntese de derivados do fluoróforo rodamina utilizando metodologias mais limpas e mais eficientes", Science Faculty – Universidade do Porto (2011).

Vasco Nuno Maia Almeida, MSc Thesis "Sintese e avaliação da actividade protectora de metabolitos do hidroxitirosol", Science Faculty – Universidade do Porto (2011).

Sandra Cristina das Neves Pereira da Costa, MSc Thesis "Síntese de metabolitos do 3,4-DHPEA-EDA" Science Faculty – Universidade do Porto (2011).

Fábio David Gouveia Félix Raimundo, MSc Thesis "Síntese e estudo da agregação de tensioactivos derivados de serina: rumo a novos lipossomas biocompatíveis" Science Faculty – Universidade do Porto (2011).

Maria João Castro Gouveia, MSc Thesis "Desenvolvimento de novos inibidores da ITK para o combate ao vírus HIV-SIDA" Science Faculty – Universidade do Porto (2011).

Sandra Cristina das Neves Pereira da Costa, MSc Thesis "Síntese de metabolitos dos polifenóis do azeite" Science Faculty – Universidade do Porto (2011).

Liliane A. M. Junqueira, MSc Thesis "Síntese compostos derivados de aminoácidos e tripéptidos lipofílicos potencialmente bioactivos" Science Faculty – Universidade do Porto (2011).

André Manuel Ferreira Fonseca, MSc Thesis "Desenvolvimento e Estudo Computacional de Novos Inibidores da Monoaminoxidase e da Acetilcolinesterase Baseados na Estrutura da Cumarina" Science Faculty – Universidade do Porto (2011).

Pedro Henrique Gomes Soares, MSc Thesis "Síntese de Derivados de Tienopiridinas e de Tienopirimidinas como Compostos Antitumorais e/ou Antiangiogénicos" Science Faculty – Universidade do Porto (2011).

José Carlos Santos Teixeira, MSc Thesis "New mitochondria-targeted antioxidants based on cinnamic scaffold as a therapeutic solution for neurodegenerative disease" Science Faculty – Universidade do Porto (2011).

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Diana Catarina Parente Meixedo, MSc Thesis "Estudo da potencial utilização como agente de contraste em Imagem por Ressonância Magnética de novos magnetolipossomas", CENIMAT/I3N, Faculty of Sciences and Technlogy – Universidade Nova de Lisboa (2012).

Rogério Seong Chay, MSc Thesis "Synthesis of Palladium aminocarbene complexes and their application as catalysts in Suzuki-Miyaura cross-coupling reaction", (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2012).

Filipa Brito, MSc Thesis "Role of Monocarboxylate transporter 1 (MCT1) and Lactate dehydrogenase A chain (LDHA) in Acute Myeloid Leukaemia (AML)", Faculty of Sciences of Lisbon University (2012).

Vanessa Vieira, MSc Thesis “Investigation of a Novel Ferrous Homeostasis Pathway”, Faculty of Sciences of Lisbon University (2012).

Cláudia Figueira, PhD Thesis “Preparação, caracterização e optimização de novos catalisadores de oligo/polimerização de olefinas isentos de activadores de alumínio” (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2012).
Supervisor: Pedro Teixeira Gomes
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/47730/2008)

Luis Alves, PhD Thesis “Synthesis, Reactivity and applications of Zirconium and Copper Complexes Incorporating Cyclam-based ligands” (IST-UTL) Instituto Superior Tecnico – Universidade Tecnica de Lisboa (2012).
Supervisor: Ana M. Martins
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/44295/2008)

Aldino Viegas, PhD Thesis “Molecular determinants of Ligand Specificity in Carbohydrate-Binding Module: an NMR and X-ray crystallography integrated study” (FCT-UNL) Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa (2012).
Supervisor: Eurico J. Cabrita, Anjos L. Macedo e Ana Luisa Carvalho
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/35992/2007)

Gustavo Barreira, PhD Thesis “Characterization of Sol-Gel matrices with entrapped cutinase” (FCT-UNL) Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa (2012).
Supervisor: Eurico J. Cabrita, Susana Barreiros
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/34800/2007)

Filipe Freire, PhD Thesis “Integrated study by NMR and X-ray Crystallography on the analysis of the molecular interactions in heme-binding proteins” (FCT-UNL) Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa (2012).
Supervisor: Anjos L. Macedo, Maria J. Romao
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/30239/2006)

Filipa Alexandra Delgado Siopa, PhD Thesis “Modificação de proteínas e DNA por quinonas derivadas de catecolaminas” (FCT-UNL) Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa (2012).
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/39171/2007)

Maria Leonor Carvalho Morgado, PhD Thesis “Structural and functional studies of PpcA: a key protein in the electron transfer pathways of Geobacter sulfurreducens” (FCT-UNL) Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa (2012).
Supervisor: Carlos A. Salgueiro
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/37415/2007)

Paula Manuela Lopes Correia da Silva, PhD Thesis “Funcionalização regiosselectiva da sacarose e sua aplicação na síntese de novos materiais” (FCT-UNL) Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa (2012).
Supervisor: Maria Teresa Barros e Krasimira T. Petrova
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia

Rui Miguel Garcia da Costa Pinto, PhD Thesis “Síntese selectiva de moléculas com potencial interesse biológico. Desenvolvimento de metodologias sustentáveis” (FCT-UNL) Faculdade de Ciencias e Tecnologia – Universidade Nova de Lisboa (2012).
Supervisor: Maria Teresa Barros
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia

Cecilia Pinto, MSc Thesis “Insights into copper resistance in Marinobacter hydrocarboclasticus – new bacterial copper resistance system. A gene expression and regulation study”, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa (2012).

Joana Margarida Franco Dantas, MSc Thesis “Follow the red road of triheme cytochromes in Geobacter sulfurreducens”, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa (2012).

Ana Paula Nascimento Fernandes, MSc Thesis “Caracterização de um novo citocromo do tipo c que forma "nanofios" de hemos em Geobacter sulfurreducens”, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa (2012).

Ana Lucia Carvalho, PhD Thesis “Metabolic engineering of Lactococcus lactis for improved tolerance to acid stress: guidelines from in vivo NMR analysis of glucose metabolism” ITQB-UNL, Instituto de Tecnologia Química e Biológica (2012).

Ivo Saraiva, PhD Thesis “Structural and functional characterization of the gene products responsible for phototrophic iron oxidation by purple bacteria: shining light on iron oxidation” ITQB-UNL, Instituto de Tecnologia Química e Biológica (2012).

Ana Sofia Cunha, PhD Thesis “Homeostasis of mannosylglycerate and glucosylglycerate pools in microorganisms through regulation of biosynthesis and hydrolysis” Universidade de Coimbra (2012).

Andreia Isabel Sousa Almeida, PhD Thesis “Síntese e Transformação de 4-Quinolonas e Quinolinas” CICECO, Universidade de Aveiro (2012).

Nuno Miguel Malavado Moura, PhD Thesis “Síntese e Potenciais Aplicações de Novas Porfirina ß–Funcionalizadas” CICECO, Universidade de Aveiro (2012).

Andrêa Susana Cabral da Fonseca, PhD Thesis "New fluorescent analytical systems based on oxygen and nitrogen heterocycles for application as photocleavable protecting groups for solution and solid phase synthesis", (CQ/UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Susana Paula Graça Costa
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/32664/2006)

Rui Filipe Araújo, PhD Thesis “Chemical functionalization of carbon nanotubes” (CQ/UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Maria Fernanda Proença, Carlos Jorge R. Silva.
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/38318/2007)

Maria Goretti Carvalho Pereira, PhD Thesis “Dehydroamino acids as building blocks for the synthesis of new amino acid derivatives” (CQ/UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Paula M.T. Ferreira, Luís Sieuve Monteiro.
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/38766/2007)

Ana Helena Dias Bacelar, PhD Thesis “Synthesis and antitubercular activity of new nitrogen heterocyclic compounds having a hydrazide unit” (CQ/UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Maria Alice Carvalho
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/24959/2005)

Maria José Gomes Fernandes, PhD Thesis "Fused polycyclic and coumarin derivatives as fluorescent phototriggers for neurotransmitter caging" (CQ/UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Susana Paula Graça Costa, Maria do Sameiro Torres Gonçalves
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/36695/2007)

Sandra Maria Pinto Cerqueira Barros, PhD Thesis “Development and characterization of elastase inhibitor-peptides for wound dressing applications” (CQ/UM) Chemistry Center – Universidade do Minho (2012).
Supervisor: Artur Cavaco-Paulo, João Carlos Marcos, José Alberto Martins.
Financial Support: PhD grant from Fundação para a Ciência e Tecnologia (SFRH/BD/36522/2007)

Alexandra M. Fernandes Brito, MSc Thesis “Synthesis and Reactivity of pyrimidine N-oxides for synthesis of new molecules with potential biological activity”, (CQ/UM) Chemistry Center – Universidade do Minho (2012).

Hugo Ricardo Matos Viana, MSc Thesis “Synthesis of thienopyridine derivatives as potential antitumoral and/or antiangionenics”, (CQ/UM) Chemistry Center – Universidade do Minho (2012).

Tatiana Alexandra de Freitas Perdigão Dias, MSc Thesis “Synthesis of epigallocathecin-3-gallate derivatives”, (CQ/UM) Chemistry Center – Universidade do Minho (2012).

Raquel Cistina Ribeiro Mendes, MSc Thesis “Synthesis and enzymatic activity of 1-N-carboxamide derivatides of 1-azafagomine and 5-epi-1-azafagomine”, (CQ/UM) Chemistry Center – Universidade do Minho (2012).

Juliana Justino de Andrade, MSc Thesis “Self-assembled noncovalent hydrogels based on dehydrodipeptides”, (CQ/UM) Chemistry Center – Universidade do Minho (2012).

Janaína Solange Gonçalves, MSc Thesis “Gold nanoparticles and quantum dots functionalized with Gd3+ chelates as contrast agents for medical imaging”, (CQ/UM) Chemistry Center – Universidade do Minho (2012).

Jorge Manuel Dias Fernandes, MSc Thesis “Transition metal chelates as potente new anticancer agents”, (CQ/UM) Chemistry Center – Universidade do Minho (2012).

Iva Luzia Reis Fernandes, PhD Thesis “Hemisíntese, biodisponibilidade e propriedades biológicas de pigmentos antociânicos e metabolitos” Science Faculty – Universidade do Porto (2012).
Supervisor: Nuno Mateus

Susana Soares, PhD Thesis “Influência dos compostos polifenólicos no sabor dos alimentos: relação entre a sua estrutura e a capacidade de interação com proteínas da saliva e recetores do sabor” Science Faculty – Universidade do Porto (2012).
Supervisor: Victor de Freitas

Rui Gil da Costa Oliveira, PhD Thesis “Studies on the biopathological actions of Pteridium aquilinum” Instituto Ciencias Biomedicas Abel Salazar – Universidade do Porto (2012).
Supervisor: Carlos Lopes, Margarida M. S. M. Bastos, Paula Oliveira.

Clara Isabel Barbosa Rodrigues Pereira, PhD Thesis “Nanostructured Materials and Nanoparticles as Supports for the Design of Novel Hybrid Catalysts” Science Faculty – Universidade do Porto (2012).
Supervisor: Carlos Lopes, Margarida M. S. M. Bastos, Paula Oliveira.

Sara Isabel Gonçalves Pereira, MSc Thesis "Desenvolvimento de Novos Neuroprotetores Análogos da Rasagilina como uma Nova Estratégia Terapêutica para as Doenças de Parkinson e Alzheimer", Science Faculty – Universidade do Porto (2012).

Joana de Fátima Matias Rodrigues, MSc Thesis "Síntese de derivados acilados do anti-inflamatório Naproxeno", Science Faculty – Universidade do Porto (2012).

Miguel Ángel González Fernández, MSc Thesis "Síntese de péptidos antimicrobianos com potencial atividade contra H. Pylori", ERASMUS Program, Universidade de Valencia (2012).

Ester Sofia Benfeito, MSc Thesis "Desenvolvimento de novos antioxidantes baseados no ácido cinâmico", Science Faculty – Universidade do Porto (2012).

Ana Catarina Oliveira, MSc Thesis "Desenvolvimento de novos antioxidantes baseados no ácido benzóico", Science Faculty – Universidade do Porto (2012).

José Manuel Costa Dias, MSc Thesis "Promoção da solubilidade de cromonas recorrendo ao uso de ciclodextrinas", Science Faculty – Universidade do Porto (2012).

Ricardo Nuno Quesado Alves, MSc Thesis "Eficiência de antioxidantes na estabilização do Biodiesel", Instituto Superior de Engenharia do Porto (2012).

Nelson Augusto Esteves Preto, MSc Thesis "Avaliação da influência de antioxidantes na estabilização de Biodiesel", Instituto Superior de Engenharia do Porto (2012).

Sara Carvalhal Figueiredo, PhD Thesis "Innovative Platforms for MRI-based Applications" Faculty of Science and Technology, and Center of Neurosciences and Cell Biology, University of Coimbra (2012).
Supervisor: Carlos F.G.C.Geraldes, Silvio Aime, Univ. Torino (Italy)

Inês Ribeiro Violante, PhD Thesis "The neurobiological basis of Neurofibromastosis type 1: new insights into brain structure, function and neurochemistry" Faculty of Medicine, University of Coimbra (2012).
Supervisor: Miguel Castelo Branco, Carlos F.G.C.Geraldes

Ivan Viegas, PhD Thesis "Sources of Blood Glucose and Liver Glycogen in the Seabass: Implications for Carbohydrate Metabolism in Fish" Faculty of Science and Technology, and Center of Neurosciences and Cell Biology, University of Coimbra (2012).
Supervisor: JG Jones, Rui Carvalho, Miguel Pardal

Rui Pedro Ferreira Lopes, MSc Thesis "Cisplatin Interplay with DNA bases: a molecular view", Faculty of Science and Technology, University of Coimbra (2012).

Filipa Vanesssa Carvalho Simões, MSc Thesis "Noninvasive Analysis of Hepatic Acetyl-CoA by Chemical Biopsy", Faculty of Science and Technology, University of Coimbra (2012).