

Global Scientific Report 2014

Funchal, January 2015













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THE RESEARCH UNIT IS SUPPORTED BY

FCT Fundação para a Ciência e a Tecnologia

MINISTÉRIO DA EDUCAÇÃO E CIÊNCIA

FCT-IP Research Unit Number: 674

(CHEM-Madeira-Funchal - PEst-OE/QUI/UID0674/2014)

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"A Química é Divertida/Chemistry is Fun": http://cqm.uma.pt/quimicadivertida



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GOVERNANCE STRUCTURE I

EXECUTIVE COMMITTEE

João Rodrigues | SCIENTIFIC COORDINATOR

Helena Tomás | MATERIALS GROUP DIRECTOR

Paula Castilho | NATURAL PRODUCTS GROUP DIRECTOR

MANAGEMENT & COMMUNICATION MEDIA

Emília Pimenta | PROJECT MANAGER
Énio Freitas | SECRETARIAT

Paula Andrade | ADMINISTRATIVE AND TECHNICAL STAFF
Hernâni Zao | COMMUNICATION DIRECTOR

PERMANENT EXTERNAL SCIENTIFIC ADVISORY COMMISSION

| Professor José Martinho Simões

Full Professor FCUL- Faculdade de Ciências, Universidade de Lisboa, Portugal

| Professor Gordon Cragg

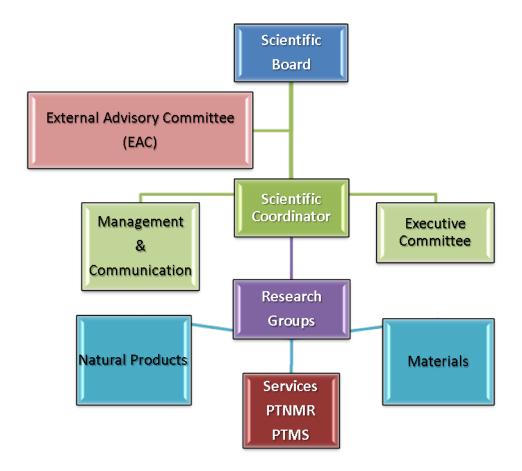
Retired Chief, Natural Products Branch, National Cancer Institute, USA

| Professor Makoto Fujita

Full Professor, Department of Applied Chemistry, University of Tokyo, Japan



ORGANIZATIONAL STRUCTURE I





VISION AND MISSION I

OUR VISION/MISSION

CQM envisages becoming a renowned research institution in the field of Natural Products and Materials, thus contributing for the development of the University of Madeira (UMa), the Madeira Archipelago, and the social and economic growth and cohesion within Portugal and Europe. CQM aims to become a R&I centre where new fundamental knowledge is produced and solutions to real world problems are created with potential to be converted into practicable, scalable, and marketable products. Also, CQM would like to generate a R&I environment adequate for advanced training, simultaneously fostering the attraction of new and outstanding students.

WORKING AREAS AND RESEARCH GROUPS

CQM is organized in two interdisciplinary research groups — **Materials** and **Natural Products** — developing its R&D activities in the fields of Analytical Chemistry, Food Chemistry, Health, Materials, Molecular Modelling, Nanochemistry and Phytochemistry.

OUR LOGO

The CQM logo is composed of different colored petals representing different areas of chemistry and biochemistry that work together to improve the scientific knowledge and contribute to the well-being of Society.

A permanent quest for sustainable knowledge and excellence in the field of Natural Products and Materials



CQM COMMITMENTS AND PRINCIPLES

CQM follows the rules of Fundação para a Ciência e a Tecnologia (FCT-IP), the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers (Commission Recommendation, Brussels, 11.3.2005, 2005/251/EC), being committed with the principle of equity in employment and selection based on merit.

CQM follows the Code of Conduct from the University of Madeira and is strongly engaged with all the European regulation related with the ethical, legal and social aspects (ELSA) and governance of nanotechnology, namely with the COMMISSION RECOMMENDATION of 07/02/2008. CQM also voluntary follows the Code of Conduct for responsible Nanosciences and Nanotechnologies research and the opinion of the European Group on Ethics in Science and New Technologies concerning the ethical aspects of Nanomedicine.

Part of the research that is being conducted at CQM is in close collaboration with the local Hospital. In particular, adult human stem cells and other human tissue samples are being used in the studies with authorization of the Hospital Ethical Committee and respecting the National and European rules.



OBJECTIVES AND ACHIEVEMENTS 2014

1. UNIT DESCRIPTION

CQM is a research unit launched in 2004, hosted by the University of Madeira (UMa), Madeira Island, an outermost region of Europe. While having scientific and strategic autonomy, CQM is integrated into the Competence Center of Exact Sciences and Engineering (CCESE), a university structure that aggregates the previous Departments of Chemistry, Mathematics and Engineering, and Physics, where it plays a pivotal role in undergraduate and advanced training activities. CQM activities are also relevant to key stakeholders at Madeira, like the industrial and educational sectors. It should be highlighted that the CQM is the only FCT research unit in Madeira and Azores archipelagos with a strong knowhow in Chemistry and Biochemistry and regularly evaluated by an international panel of experts.

At the end of 2014, the CQM's team was composed of 57 researchers:

- a) 11 PhD members corresponding to the permanent staff (8 from the CCESE and the Competence Center of Life Sciences, 1 from an R&D governmental lab, 1 contracted in the scope of the FCT Science 2008 programme, and 1 sponsored by the Santander Totta Bank (Invited Chair in Nanotechnology));
- b) 4 Post-Doc fellows;
- c) 42 registered collaborators/Students (including 9 researchers holding a Master's degree, 11 PhD Students, 13 Master Students);
- d) 15% were expatriates and 51% were women.

Since it was launched, CQM has two well established and interdisciplinary research groups (Natural Products Group (NPG) & Materials Group (MG)) sharing a state of art research infrastructure, and developing research in the fields of Analytical Chemistry, Food Chemistry, and Materials/Nanomaterials for biomedical applications. The NPG has an extensive expertise in Chromatography and Mass Spectrometry-based identification and structural elucidation of biologically active low molecular weight molecules. LCMS-based methodologies development in natural products, natural small molecules screening and target analysis, metabolites or biomarker discovery, quantitative determination of small molecules in biological and environmental matrixes and speciation analysis of trace elements, have been key topics of research. The MG is the only one in Portugal with a strong knowledge of dendrimer chemistry (synthesis, characterization and applications), mainly developing its work in the following areas: metallodendrimers, hybrid dendrimer-based nanomaterials, functionalization of dendrimers/nanomaterials for biological targeting (cancer cells, stem cells), inorganic nanoparticles templated by dendrimers. The applications involve drug/gene delivery, bioimaging and theranostics.

The research unit is managed by: a) The Scientific Coordinator (SC); b) The Scientific Board (SB); and c) The Executive Committee (EC). The SC is a PhD permanent member of the staff and is responsible for representing the unit in all R&D aspects. The SC is elected by the SB for a period of 2 years. The SB is composed by all the PhD permanent members of the staff and

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establishes the main rules for the CQM management, along with the scientific strategic plan for the unit. The EC is formed by the SC and two other members of the SB (usually, the 2 group directors), and has the role of implementing the decisions of the SB, of monitoring the progress of the research activities, and of organizing network type activities among the members. The two interdisciplinary research groups of CQM (Natural Products & Materials) are led by a senior PhD permanent member of the staff (group director/principal investigator) appointed by the Scientific Board. The management and strategic plan of CQM have also in consideration the opinion of a Permanent External Scientific Advisory Commission (PESAC) appointed by the SB.

The coordination of special activities/projects (such as post-graduate courses, outreach science actions, etc.), maintenance and management of important equipment, such as the 400MHz NMR and LCMSMS equipment, as well as safety and lab space management can be assigned to specific CQM members.

CQM also benefits from the work of two administrative staff members belonging to UMa (on a part-time basis) for the financial management of R&D projects (including the FCT-IP pluriannual budget).

For their research activities, the members of CQM share 5 specific research labs (Biochemistry & Cellular Culture Lab; Molecular Modelling Lab; Analytical Chemistry & Enology Lab; Molecular Materials & Coordination Chemistry Lab; Organic Chemistry & Natural Products Lab), 1 polyvalent lab, and the NMR and MS services labs, in a total area of 700 m². These last labs make part of the National NMR and MS networks (http://ptnmr.dq.ua.pt/ & http://ptnmr.dq.ua.pt/ & http://ptnmr.dq.ua.pt/ & http://ptnmr.dq.ua.pt/ & http://ptnmr.dq.ua.pt/).

Although CQM achieved a classification of 22.5 (in 25) in the last FCT evaluation exercise (2013), CQM's pluriannual base funding was based on the one performed in 2008 (the unit was classified as "Good"). As such, the funds attributed by FCT in the year 2014, only reached the total amount of €33,290 (15% of this value corresponds to University overheads). CQM's financial strategy is to primarily prioritize the common interests of the whole Unit (equipment maintenance, as well as common consumables, such as gases and cryogenic liquids, etc.), and if possible, to invest in the acquisition of new equipment. The remaining budget is distributed among the permanent PhD staff members, according to their requirements. In 2014, roughly 71.4% of the annual budget was spent on common expenses.

2. GENERAL OBJECTIVES

Based on the expertise of the CQM members, the geographical location of the unit, and the strategic areas defined by UMa, by the National and the Regional Governments (nanotechnology and health sciences), as well as by the European Union, CQM decided to direct efforts towards applied research with high local impact (Natural Products, with a strong component of Analytical Chemistry) and, simultaneously, to choose a new emergent field of research to reinforce its international visibility (Materials, namely Nanomaterials for biomedical applications).

CQM's main objective is to be a leading international R&D entity in the field of Natural Products and Materials. It is also our aim to contribute to the promotion of the scientific culture among the general population, in particular the younger generation. It should be



highlighted that CQM is the only existent research unit in all of the Madeira Archipelago with a strong knowhow in Chemistry.

In order to achieve these general objectives, CQM aims to:

- a) Focus the R&D activities, taking into consideration the expertise of the CQM members, the geographical location of the unit, and the strategic areas in terms of R&D activities defined for the near future by the University of Madeira, the National and the Regional Governments (nanotechnology and health sciences), as well as the European Union;
- b) Strengthen the two research groups by increasing the number of PhD members, PhD students and Master students. We have a permanent open call on our website for PhD students and Post-Doc researchers; this has also been announced on international websites (e.g. Nature Jobs and the EURAXESS Jobs Portal). Indeed, over the past few years, we have submitted a large number of applications to the FCT program for "Advanced Training and Qualification of Human Resources";
- Reinforce the center with necessary/crucial equipment not yet available at our University, either through research project funding or through national programs dedicated to equipment acquisition;
- d) Establish new national and international collaborations and networking, while empowering the existing ones, with institutions and companies able to support and complement our research;
- e) Promote the ongoing research at CQM at the national and international levels;
- f) Search for funds by submitting project proposals at the national and international levels, along with other national and international partners;
- g) Reinforce the interactions between both research groups at CQM by launching more collaborative research projects;
- h) Increase and improve the number and quality of publications (Impact Factor), an objective that will certainly be fulfilled in the following years as a result of the work being performed up to now;
- Generate a R&D environment suitable for the advanced training at UMa, namely by giving the needed scientific support to the post-graduate courses offered by UMa (namely, the Master's degree program in "Applied Biochemistry" and the Master's degree program in "Nanochemistry and Nanomaterials");
- j) Be actively involved in the organization or co-organization of scientific meetings;
- k) Maintain active the ongoing projects on the popularization of science that are devoted to the general public.

3. Main Achievements – Focus On 2014

In accordance with the medium/long term objectives established and previously mentioned, the following major achievements in 2014 must be highlighted:



a) CQM was classified with 22.5 points – Very Good (in a maximum of 25) in the last evaluation conducted by FCT.

FCT opted to set up an agreement with the European Science Foundation (ESF) in order to involve this international, non-governmental organisation in the peer-review process of Portuguese R&D Units. In this scope, CQM submitted a report activity concerning the period 2008-2012 and received the visit of a panel of ESF experts in October 2014. As a result, CQM was classified with Very Good (22.5 points in a maximum of 25) — this result is pendent since CQM appealed from this classification believing that the right one should be Excellent based on work produced and on the comments of the panel of evaluators.

b) CQM was able to obtain competitive external funding that allowed an important improvement of its human and physical resources.

Beyond the budget secured for 2014 from past projects (€765,919), two new projects with European funding (Programme PCT MAC 2007-2013) were approved, providing more €87,500 for UMa (totalizing €853,419). Additionally, 4 grants (2 management science grants, 1 PhD grant supported by FCT, and 1 research grant funded by "Liga Portuguesa contra o Cancro" were approved which started in 2014 or will start in 2015).

Furthermore, as a direct result of the FCT evaluation, the pluriannual funding of FCT for the period 2015-2020 will be €120,723 per year (3.6 times more per year than previously).

c) CQM strengthened the national and international collaborations, including those with companies.

In 2014, CQM has reinforced the already existent scientific collaborations and established new partnerships with important national and international groups. These collaborations were based on research projects, bilateral agreements, scientific networks and co-supervision of PhD and post-docs students (most of the collaborations are headed by CQM). From the list of our collaborations we can highlight: Porto Univ.(INEB and IPATIMUP), Évora Univ., Azores Univ., REQUIMTE, La Laguna Univ.(Spain), Donghua Univ.(Shanghai, China), Antwerp Univ. (Belgium), Corse Univ. and Bordeaux Univ. (France), Materials Eng. Res. Inst. (Sheffield Hallam Univ., UK), and NanoScience Center (Jyväskylä Univ., Finland). CQM also has a strong relationship with the local Hospital, companies and regional Governmental R&D Labs, leading or coleading several R&D projects (e.g. Santander Bank, Madeira Wine Company, Regional Lab. of Civil Engineering, Extermínio).

CQM is a full member of the following Portuguese networks and consortiums: National NMR & MS Networks, all supported by FCT, being also a member of the National Affiliated Centre - Cambridge Structural Database consortium. At



the international level, CQM integrates the COST Action TD0802 (Dendrimers in Biomedical Applications; currently without funding), the networks BIOPHARMAC (http://www.biopharmac.eu/), and SUPRAPHONE. Furthermore, the work developed in the period under analysis also resulted in the following network participations: INDIGO-ERA NET (started in 2013); the Bilateral agreement with India "Functionalized Nano-antimalarials: Design, Synthesis and Structural Aspects" (2013-2016); the project IMBRAIN FP7-REGPOT-FP7-2012-CT2012-316137 (started in 2013); and the CYTED RED IBEROAMERICANA Project P213RT0409: Development of a vaccine against HIV(started in 2014).

d) CQM supports two MSc courses at UMa

CQM is generating the adequate R&D environment suitable for the advanced training at UMa. Namely, it gives the scientific support to the following programmes: PhD in Chemistry, MSc in Applied Biochemistry (1st ed. in 2007/2008), and MSc in Nanochemistry and Nanomaterials (1st ed. in 2012/2013; this master course enrolls students from Portugal, China, and India). During the year 2014, the PhD in Chemistry and the MSc in Applied Biochemistry, were evaluated by the A3ES (Agency for Assessment and Accreditation of Higher Education) and approved, respectively for more 3 and 5 years.

- e) CQM was able to consolidate the research within the two research groups resulting in an increase in the number and quality of the research outputs
 In 2014, CQM published 24 papers in peer-reviewed journals with IF which represented around 24% of the total papers published by UMa. Fourteen of the 24 papers were published in journals with an IF higher than 3.5.
 In detail:
 - 1. Papers in peer-reviewed journals with IF: 24 (plus 14 accepted). 16 of the total papers were published in co-authorship with teams from other countries (degree of internationalization¹: 75%);
 - 2. Book and book chapters: 5 book chapters;
 - 3. Papers in peer-reviewed journals without IF: 3;
 - 4. Conference proceedings: 1;
 - 5. Technical and scientific reports: 2;
 - 6. Oral communications: 45 (17 in international conferences);
 - 7. Seminars at other universities: 8;
 - 8. Posters: 33 (31 in international conferences);
 - 9. PhD Thesis Defenses: 0; Master Thesis Defenses: 8;
 - 10. Press articles and TV news: 20 (15 min in TV prime time);
 - 11. Number of international conferences and advanced schools organized or co-organized by CQM team members: 2;
 - 12. Number of national conferences or advanced schools organized or coorganized by CQM team members: 1;

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¹Papers published in collaboration with teams of other countries.



- 13. Number of short courses organized by CQM team members: 1;
- 14. Number of visiting fellows: (Brazil (2), Hungary (2), France (1), Sweden (2), United Kingdom (1), Germany (2), Spain (2), Israel (1), Romania (1));
- 15. Number of advanced training students: 11 PhD Students; 11 Master Students;
- 16. Number of networks having the participation of CQM: 11.

CQM's evolution can be summarized by the following Facts and Figures for the period of 2011-2014:

- Number of PhDs: **2011** (20); **2012** (17); **2013** (16); **2014** (15)
- Number of PhD students: **2011** (8); **2012** (9); **2013** (11); **2014** (11)
- Number of Master students: **2011** (10); **2012** (7); **2013** (17); **2014** (13)
- Publications with IF: **2011** (29); **2012** (43); **2013** (41); **2014** (24)
- Average IF: **2011** (4.3); **2012** (4.4); **2013** (4.5); **2014** (4.3)
- f) CQM organized the the Materials Group and the 9th Annual Meeting
- g) CQM arranged the 7th edition of NanoSchool



ACTIVITIES

1. INTEGRATIVE/MULTIDISCIPLINARY ACTIVITIES DURING 2014

As a relatively small unit, the contact between both research groups is easy, promoted and fundamental for the growth and consolidation of the research center. In 2014, the CQM members from the Materials Group and the Natural Products Group worked together in:

- a) The 1st Annual CQM Meeting (in the previous years two separated meetings were performed, one per research group): 31th January to 1st February involving a total of 32 oral communications (open to all academia).
- b) A series of conferences done in the scope of the commemoration of the 10 Years of CQM, namely:
 - "New Nanomaterials Based on Biodegradable Supramolecular Nanohydrogels for Applications in Drug Delivery", Prof. Cátia C. C. Ornelas Megiatto, Chemistry Institute, University of Campinas – UNICAMP, Campinas, Brazil (7th January).
 - "Interlocking Molecules: A True Way to Deliver the Promises of Nanotechnology or Another Story for Suckers...", Prof. Jackson Megiatto, Chemistry Institute, University of Campinas – UNICAMP, Campinas, Brazil (7th January).
 - "Cavities in PAMAM G5-NH2 dendrimer. How does NMR see?", Prof. István Bányai, Department of Colloid and Environmental Chemistry, Faculty of Science, University of Debrecen, Hungary (19th February).
 - "Nanopaprika.eu Spicy world of nanoscience" scientific social network for nanotechnology researchers", Dr. András Paszternák, The International NanoScience Community, Hungary (www.nanopaprika.eu) (7th May).
 - "NMR metabolomics in the BETULA project, biomarkers for Alzheimer's disease", Dr. João Figueira, Department of Pharmacology and Clinical Neuroscience, Umeå University, Umeå, Sweden (16th July).
 - "Bioactive lipids profiling by LC/MS", Dr. Sandra Gouveia Figueira, Department of Chemistry, Umeå University, Umeå, Sweden (16th July).
 - "Nanomedicines: Fact of Fiction?", Prof. Ruth Duncan, Professor Emerita, Cardiff Univ., United Kingdom (8th October).
- c) The "CQM Insights" (the CQM newsletter, edited in English and in Mandarin).
- d) The 1st Science Communication Course, 12-13 December (by Dr. Hernâni Zão, Communication Director of CQM); this Science Communication Short Course was developed to input an ascending dynamics between the CQM's research groups, increasing the quality of education for the students and researchers.
- e) The outreach activities (science popularization activities) which are described in the next section).



- f) Supervision of Master (Z. Qiao) and PhD students (C. Luís, Ref. SFRH/BD/97039/2013).
- g) The projects connected with the participation of CQM in the National NMR (PTNMR) and Mass Spectrometry (RNEM) networks. In the scope of the mentioned networks, one PhD technician and a technician with a Master were hired by CQM to work with the equipment and support both research groups:
 - Node CQM/UMa: Approved by FCT: € 144 464 (2010-2014). Principal Investigator: João Rodrigues.
 - Node CQM/UMa: Approved by FCT: € 99 952 (2009-2014). Principal Investigator: João Rodrigues.
- h) The management/sharing/maintenance of equipment and Lab spaces.

2. OUTREACH ACTIVITIES DURING 2014

The important role of CQM in boosting science in Madeira archipelago through several scientific outreach activities that have the objective of promoting and disseminating science amongst the general public (the youngsters in particular) should be highlighted.

The scientific outreach activities that were carried out by our research center and team members in 2014 included:

- a) The two days event, integrated in the National Week of Science and Technology (in November), "A Química é Divertida /Chemistry is Fun" (http://cqm.uma.pt/quimicadivertida)², organized at CQM labs, involved several chemistry related activities designed for the general public, and was visited by 500-600 persons.
- b) The "Ocupação Científica de Jovens nas Férias/ Science during holidays" involved the participation of 15 high school students in a period of training at CQM (7-11 July); this activity was supported by the Agência Nacional para a Cultura Científica e Tecnológica (ANCCT) - Ciência Viva.
- c) "Estágios de Verão no CQM/Summer periods of training at CQM" organized in July (several undergraduated students were enrolled in this training program); here, the students had the opportunity to become familiar with the routine of lab research, learn new techniques, gain new skills and develop new attitudes to overcome common and advanced research problems. In addition, the students had the possibility to learn more about the research performed at CQM.

Beyond the mentioned activities, CQM received visits from high school students (about 10 groups of students).

²"The Chemistry is Fun" initiative was started in 1995 at the former Chemistry Department, by the founder member of CQM, Paula Castilho. Global Scientific Report 2014



Our privileged way to disseminate CQM's activities is through our website (http://cqm.uma.pt), in English and Portuguese. We also make use of Twitter (http://twitter.com/UMa_CQM; in December 2014 we were followed by 251 persons or organizations, mainly from academia) and Facebook (http://on.fb.me/GCe7kN; followed by 430 "friends"). Furthermore, we have a regular press release service, a CQM flyer and a Facts and Figures report (continuously updated) to be distributed during the events organized by CQM.

CQM also often makes the news in the regional and national media. In 2014, ca. 20 short articles (interviews in newspapers and in specialized scientific websites) and TV news were published. The regional TV channel usually covers all our activities (conferences, science popularization actions, etc.). Overall, CQM's activities obtained a total estimated time of 15 minutes on prime time news on the Regional TV station and more than 5 min in the Regional Radios. CQM members were also interviewed for the program "O Pátio dos Estudantes" (produced by the Student Union for the regional TV station) and for the Student Union's magazine.



SCIENTIFIC REPORT OF THE MATERIALS GROUP |

1. GROUP DESCRIPTION

• Research Group Title: (RG-Madeira-674-390) - Materials Group

• Principal Investigator: Helena Maria Pires Gaspar Tomás

• Research Area: Materials Chemistry

• Home Institution: Universidade da Madeira

2. FUNDING, SOURCE(S), DATES

Available funding for 2014 | €253,557

Main Ongoing Projects and Grants headed by the Group (FCT funded):

- €197.616 (€197.616 for CQM): FCT funded. PTDC/CTM-NAN/1748/2012. 2013-2015; PI: Xiangyang Shi (DENDIMAGE Development of Novel Dendrimer-Based Nanoparticles for Dual Mode Computed Tomography and Magnetic Resonance);
- €151.251 (€80.193 for CQM): PTDC/CTM-NAN/112428/2009. 2011-2014; PI: Helena Tomás (DENDRIMAT – New materials for drug/gene delivery based on the self-assembly of dendrimer-chitosan-single stranded DNA);
- €156.808 (€156.808 for CQM): FCT funded. PTDC/CTM-NAN/116788/2010. 2012-2015; PI: Yulin Li (SELFNANO Self-assembled Nanoparticles based on PEG-PLA-dendrimer building blocks for dual gene/drug delivery);
- €8.100 (€8.100 for CQM): Bilateral agreement with India "Functionalized Nanohybrid Antimalarial Targets: Design, Synthesis and Structural Aspects of Novel Metal Complexes as Inhibitors of Plasmepsin I and Plasmepsin II"; 2013-2016. Head of the Portuguese group: João Rodrigues
- €47.040 (PhD grant): SFRH/BD/65036/2009. (Manuel Jardim)
- €47.040 (PhD grant): SFRH/BD/82361/2011. 2012-2015 (Freddy Rodrigues)
- €47.040 (PhD grant): SFRH/BD/87465/2012. 2013-2016 (Rita Castro)
- €47.040 (PhD grant): SFRH/BD/88721/2012. 2013-2016 (Mara Gonçalves)
- €53.820 (Post-Doc grant): SFRH/BPD/75420/2010. 2011-2014 (Shili Xiao)

Ongoing Projects with the participation of the Materials Group:

- €199,272 (€4,680 for CQM): FCT funded. PTDC/QEQ-MED/0905/2012. 2013-2015; Team member: Miguel Fernandes (Optimization of p-glycoprotein modulators and insights into the efflux mechanism);
- €22.450 (€9.380 for CQM): CYTED RED IBEROAMERICANA Project P213RT0409: Development of a vaccine against HIV (started in 2014). Head of the Portuguese group: João Rodrigues.

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Projects and grants to be started in 2015:

• €47.040 (PhD grant): SFRH/BD/102123/2014. 2015-2018 (Dina Maciel)

3. OBJECTIVES AND ACHIEVEMENTS

3.1 Objectives

For the coming years, the group established as its main objective to focus on research in the field of new materials (in particular, molecular and nanomaterials) that are designed and produced with specific applications in mind, namely in the areas of nanomedicine and optoelectronics. Taking advantage of a team of researchers with complementary expertise and concurrent interests (capable of connecting theory, computation and experimental work in a cohesive manner), the idea is to launch projects addressing outstanding scientific questions and technological issues, with clear objectives and an applied focus. In this scope, the objectives include the conception of new materials, processes and software related to the applications envisaged, as well as the understanding of the chemical foundations of those materials and processes. The group aims to critically question results and propose innovative ways to solve problems, to perform the highest quality research in an ethically responsible manner, to communicate findings to laypeople and experts and to promote the transfer of knowledge and technology.

In relation to the mentioned scientific objectives, the group established for 2014 and subsequent years the following measurable goals:

- To enhance the scientific output of the team, *i.e.*, the number of publications (in international peer-reviewed journals) and their impact factor;
- To increase the number of researchers (namely, Post-Doc, Master and PhD students);
- To obtain more funding (from national and European sources), especially to acquire scientific equipment necessary for the characterization of materials, particularly nanomaterials;
- To strengthen the internationalization of the team by launching new collaborative projects with institutions and universities abroad, by organizing/co-organizing scientific meetings, workshops and schools and by integrating the team into international scientific networks.

3.2 Main Achievements

At the end of 2014, the group consisted of 27 members: 10 PhDs (8 members from the host institution and 2 Post-Doc researchers), 9 researchers holding a Master's degree, 5 PhD students (FCT funded), and 3 Master Students. In 2014, two students from Donghua University (China) also worked at the Materials Group in the scope of collaborative projects (Zhu Jingyi, PhD student, and Zhe Wang, a master student).



In the period 2014, the main achievements of the Materials Group can be summarized as follows:

- a) The group published 14 papers in journals with impact factor (the average impact factor was 4.3 (IF: 2013³) and the degree of internationalization was 100%); 5 other papers were accepted for publication and more 5 papers were submitted; 1 international proceeding and 1 book chapter were also published;
- b) The group presented a total of 28 oral presentations (8 in international meetings, including 1 keynote lecture and 2 Invited oral communications) and 3 poster presentations in international scientific meetings;
- c) Based on the knowhow already existent at CQM in the field of nanomaterials, the members of the Materials Group actively participated in the Master course on "Nanochemistry and Nanomaterials" and the Master course in Applied Biochemistry which were approved by A3ES (Agency for Assessment and Accreditation of Higher Education);
- d) Prof. Serge Mignani (from the University of Paris Descartes, France) visited the group to discuss research work and give lessons to the Master in Nanochemistry and Nanotechnology (November, 2014);
- e) Six students concluded their Master's degrees (Marisol Gouveia, Dina Maciel, Tiago Fernandes, Khirtiga Ramalingan, Xuedan He, Akudari Shekar);
- f) One more PhD. grant was approved by FCT (Dina Maciel, ref. SFRH/BD/102123/2014).

4. DISTINCTIONS, AWARDS AND MERITS

- The paper: Dina Maciel D., Figueira P., Xiao S., Shi X., Hu D., Rodrigues J., Tomás H., Li Y.. Redox-responsive Alginate Nanogels with Enhanced Anticancer Cytotoxicity; *Biomacromolecules* 2013, 14, 3140–3146; was highlighted by the Portuguese Association for Cancer Research (http://www.aspic.pt/en/noticias/madeira-chemistry-research-centre-develops-nanogels-delivery-anticancer-drugs).
- Xiangyang Shi is editorial board member of the journal "ISRN Spectroscopy" (since 2011);
- Helena Tomás belongs to the Editorial Board of the journal "Biomed Research International" (Hindawi Publishing Corporation, Biomaterials area) since 2013;
- João Rodrigues is editorial board member of the following journals: "International Journal of Materials and Chemistry" (since 2011), "The Scientific World Journal" (since 2012; IF: 1.730) and of the "Mediterranean Journal of Chemistry" (since 2010; IF: 0.421).
- João Rodrigues belongs to the General Council of UMa, is one of the two members of the Finance Committee of the same Council, belongs to the Senate

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³Last impact factor available from year 2013.



of UMa and is member of the Academic Senate Committee (since 2013). He is the CQM representative at the Scientific Board of the CCESE (since 2009), and at the Scientific and Managing Board of the National Networks of Nuclear Magnetic Resonance and Mass Spectrometry (since 2007). He is, since 2009, consultant of the Deutscher Technologiedienst GmbH. He was part of the team who prepared the roadmap for Health and Wellness for the 2014-2020 action plan developed for the Regional Government, called "PIDT&I - Action Plan for Research and Technological Development and Innovation of RAM", in the framework of "Horizon 2020".

5. GROUP PRODUCTIVITY

5.1 Published Articles in Peer-Reviewed Journals (IF)

- **MP.1.** Gonçalves M.; Maciel D.; Capêlo D.; Xiao S.; Sun W.; Shi X.; Rodrigues J.; Tomás H.; Li Y.; Dendrimer-Assisted Formation of Fluorescent Nanogels for Drug Delivery and Intracellular Imaging; *Biomacromolecules* 2014, *15*, 492-499; DOI: 10.1021/bm401400r (IF: 5.788).
- MP.2. Liao H.; Liu H.; Li Y.; Zhang M.; Tomás H.; Shen M.; Shi X.; Antitumor Efficacy of Doxorubicin Encapsulated within PEGylated Poly(amidoamine) Dendrimers; *J. Appl. Polym. Sci.* 2014, *131*, 40358; DOI: 10.1002/app.40358 (IF: 1.640).
- **MP.3.** Gonçalves M.; Figueira P.; Maciel D.; Rodrigues J.; Qu X.; Liu C.; Tomás H.; Li Y.; pH Sensitive Laponite/Doxorubicin/Alginate Nanohybrids with Improved Anticancer Efficacy; *Acta Biomater*. 2014, *10*, 300-307; DOI: 10.1016/j.actbio.2013.09.013 (IF: 5.684).
- **MP.4.** Gonçalves M.; Figueira P.; Maciel D.; Rodrigues J.; Shi X.; Tomás H.; Li Y.; Antitumor efficacy of doxorubicin-loaded laponite/alginate hybrid hydrogels; *Macromol. Biosci.* 2014, *14*, 110-120; DOI: 10.1002/mabi.201300241 (IF: 3.650).
- MP.5. Wang G.; Maciel D.; Wu Y.; Rodrigues J.; Shi X.; Yuan Y.; Liu C.; Tomás H.; Li Y.; Amphiphilic Polymer-Mediated Formation of Laponite®-Based Nanohybrids with Robust Stability and pH Sensitivity for Anticancer Drug Delivery; *ACS Appl. Mater. Inter.* 2014, 6, 16687-16695; DOI: 10.1021/am5032874 (IF: 5.900).
- MP.6. Ramalhete C.; da Cruz F. P.; Mulhovo S.; Sousa I. J.; Fernandes M. X.; Prudêncio M.; Ferreira M. J. Dual-stage triterpenoids from an African medicinal plant targeting the malaria parasite. *Bioorg Med Chem*. 2014, 22, 3887–3890; DOI:10.1016/j.bmc.2 (IF: 2.951)
- MP.7. Hu D.; Huang Y.; Liu H.; Wang H.; Wang S.; Shen M.; Zhu M.; Shi X.; The Assembly of Dendrimer-Stabilized Gold Nanoparticles onto Electrospun Polymer Nanofibers for Catalytic Applications. *J. Mater. Chem. A* 2014, *2*, 2323–2332; DOI: 10.1039/C3TA13966B. (IF: 6.626)
- MP.8. Wang S.; Zhu J.; Shen M.; Zhu M.; Shi X.; Poly(amidoamine) Dendrimer-Enabled Simultaneous Stabilization and Functionalization of Electrospun Poly(γ-glutamic acid) Nanofibers. *ACS Appl. Mater. Interfaces* 2014, *6*, 2153–2161; DOI: 10.1021/am405273v (IF: 5.008).
- MP.9. Zhang M.; Guo R.; Kéri M.; Bányai I.; Zheng Y.; Cao M.; Cao X.; Shi X.; Impact of Dendrimer Surface Functional Groups on the Release of Doxorubicin from



- Dendrimer Carriers. *J. Phys. Chem. B* 2014, *118*, 1696–1706; DOI: 10.1021/jp411669k (IF: 3.607).
- MP.10. Liu H.; Wang H.; Xu Y.; Shen M.; Zhao J.; Zhang G.; Shi X.; Synthesis of PEGylated Low Generation Dendrimer-Entrapped Gold Nanoparticles for CT Imaging Applications. *Nanoscale* 2014, *6*, 4521-4526; DOI: 10.1039/c3nr06694k (IF: 6.233).
- MP.11. Liu H.; Wang H.; Xu Y.; Guo R.; Wen S.; Huang Y.; Liu W.; Shen M.; Zhao J.; Zhang G.; Shi X.; Lactobionic Acid-Modified Dendrimer-Entrapped Gold Nanoparticles for Targeted CT Imaging of Human Hepatocellular Carcinoma. *ACS Appl. Mater. Interfaces* 2014, *6*, 6944–6953; DOI: 10.1021/am500761x (IF: 5.008).
- MP.12. Liu W.; Wen S.; Jiang L.; An X.; Zhang M.; Wang H.; Zhang Z.; Zhang G.; Shi X.; PLGA hollow microbubbles loaded with iron oxide nanoparticles and doxorubicin for dual-mode US/MR imaging and drug delivery. *Curr. Nanosci.* 2014, *10*, 543-552; DOI: 10.2174/1573413710666140429223927 (IF: 1.356).
- MP.13. Fu F.; Zhu J.; Wen S.; Shen M.; Shi X.; Multifunctional lactobionic acid-modified dendrimers for targeted drug delivery to liver cancer cells: Investigating the role played by PEG spacer. *ACS Appl. Mater. Interfaces* 2014, *6*, 16416–16425; DOI: 10.1021/am504849x (IF: 5.900).
- MP.14. Stockler-Ipsiroglu S, van Karnebeek C, Longo N, Korenke GC, Mercimek-Mahmutoglu S, Marquart I, Barshop B, Grolik C, Schlune A, Angle B, Caldeira Araújo H, Coskun T, Diogo L, Geraghty M, Haliloglu G, Konstantopoulou V, Leuzzi V, Levtova A, MacKenzie J, Maranda B, Mhanni AA, Mitchell G, Morris A, Newlove T, Renaud D, Scaglia F, Valayannopoulos V, van Spronsen FJ, Verbruggen KT, Yuskiv N, Nyhan W, Schulze A Guanidinoacetate methyltransferase (GAMT) deficiency: Outcomes in 48 individuals and recommendations for diagnosis, treatment and monitoring. *Mol. Genet. Metab.* 2014, 111: 16-25 DOI: 10.1016/j.ymgme.2013.10.018 (IF: 2.827).

5.2 Book Chapters

MBC.1. Pêgo, A.P.; Moreno, P.; Castro, R.; Tomás, H.; Nucleic acid delivery mediated by polysaccharide-based vectors. In: Carbohydrates Applications in Medicine, M.H. Gil (ed.), Research Signpost/Transworld Research Network, (2014). ISBN: 978-81-308-0523-8.

5.3 Proceedings With Peer Review

MPPR.1. H Caldeira Araújo, A Pimenta, I Rivera, R Castro, I Tavares de Almeida; The onecarbon metabolism: evaluation of B-vitamin status and genetic factors on plasma homocysteine and methylmalonic acid levels in children and adolescent control groups. *J. Inherit. Metab. Dis.* 2014, 37(1) (IF: 4.138)

5.6 Accepted Papers in Peer-Reviewed Journals



- MAP.1. Xiao S.; Castro R.; Rodrigues J.; Shi X.; Tomás H.; PAMAM Dendrimer/pDNA Functionalized-Magnetic Iron Oxide Nanoparticles for Gene Delivery; *J. Biomed. Nanotech.* 2015, *11*, 1370-1384; DOI: 10.1166/jbn.2015.2101 (IF: 7.578).
- **MAP.2.** Wang Z.; Zhao Y.; Luo Y.; Wang S.; Shen M.; Tomás H.; Zhu M.; Shi X.; Attapulgite-doped electrospun poly(lactic-co-glycolic acid) nanofibers enable spontaneous osteogenic differentiation of human mesenchymal stem cells; *RSC Adv.* 2015, 5, 2383-2391 (IF: 3.708).
- MAP.3. He X.; Alves C.S.; Oliveira N.; Rodrigues J.; Zhu J.; Bányai I.; Tomás H.; Shi X.; RGD peptide-modified multifunctional dendrimer platform for drug encapsulation and targeted inhibition of cancer cells; Colloid. Surface. B 2015; 125, 82-89 (IF: 4.287).
- MAP.4. Hou W.; Guo R.; Wen S.; Wang S.; Shi X.; Partially acetylated dendrimerentrapped gold nanoparticles with reduced cytotoxicity for gene delivery applications. *J. Nanosci. Nanotechnol.* 2015, 15, 4094-4105; DOI:10.1166/jnn.2014.9618 (IF: 1.339).
- **MAP.5.** Qiao Z.; Shi X.; Dendrimer-based molecular imaging contrast agents. *Prog. Polym. Sci.* 2014, DOI: 10.1016/j.progpolymsci.2014.08.002 (IF: 26.854).

5.7 Submitted Papers to Peer Review Journals

- **MSP.1.** Li Y.; Maciel D.; Rodrigues J.; Shi X.; Tomás H.; Biodegradable Polymer Nanogels for Drug/Nucleic Acid Delivery (*submitted*)
- **MSP.2.** Leiro V.; Garcia J.; Tomás H.; Pêgo A.P.; The Present and the Future of Degradable Dendrimers and Derivatives in Theranostics (*submitted*).
- **MSP.3.** Kong L.; Alves C.S.; Hou W.; Tomás H.; Shi X.; RGD Peptide-Modified Dendrimer-Entrapped Gold Nanoparticles Enable Highly Efficient and Specific Gene Delivery to Stem Cells (*submitted*).
- **MSP.4.** Camacho C.; Mesquita J.C.; Rodrigues J.; Electrodeposition of polyaniline on self-assembled monolayers on graphite for the voltammetric detection of Iron (II) (submitted).

5.8 Thesis

- **MTH.1.** Fernandes T.; Synthesis of FITC-PAMAM conjugates for *in vitro* cell studies. Thesis presented to obtain the Master degree, Universidade da Madeira, 2014. Supervisor: João Rodrigues, co-supervisor: Helena Tomás.
- MTH.2. Ramaligam K.; Gene delivery using dendrimer/pDNA complexes immobilized in electrospun nanofibers by the LbL technique. Thesis presented to obtain the Master degree, Universidade da Madeira, 2014. Supervisor: Helena Tomás, co-supervisor: Shili Xiao.
- **MTH.3.** He, X.; RGD-modified dendrimers for drug encapsulation and targeted inhibition of tumor cells. Thesis presented to obtain the Master degree, Universidade da Madeira, 2014. Supervisor: Xiangyang Shi, co-supervisor: Helena Tomás.



- **MTH.4.** Shekar, A.; Low Generation Degradable Dendrimer Nanoclusters for Delivery of Anti-cancer Drug. Thesis presented to obtain the Master degree, Universidade da Madeira, 2014. Supervisor: Yulin Li, co-supervisor: João Rodrigues.
- **MTH.5.** Gouveia, M.; Preparation of low-generation metallodendrimers using nitrile-functionalized poly(alkylidenamines) dendrimers: cytotoxicity studies in cancer cell lines. Thesis presented to obtain the Master degree, Universidade da Madeira, 2014. Supervisor: João Rodrigues, co-supervisor: Helena Tomás.
- **MTH.6.** Maciel, D.; Cell-responsive nanogels for anticancer drug delivery. Thesis presented to obtain the Master degree, Universidade da Madeira, 2014. Supervisor: Yulin Li, co-supervisor: Helena Tomás.

5.9 Abstracts in International Scientific Meetings

5.9.1 Oral Communications

- **MOCI.1.** Alves C.S., Rodrigues J., Tomás H.; Dendrimers in bioimaging and therapeutics; Workshop Nano14 Shaping the Future; Lisbon, Portugal; 10th October, 2014.
- MOCI.2. Castro R., Santos J.L., Gonçalves M., Rodrigues J., Tomás H.; Antisense Therapy: Oligonucleotide Delivery Systems Based on Fatty-acid Functionalized PAMAM Dendrimers; 1st International Conference on Emerging Trends of Nanotechnology in Drug Discovery; New Delhi, India, 2014. (Invited oral presentation)
- MOCI.3. Gonçalves M., Figueira P., Maciel D., Rodrigues J., Qu X., Liu C., Tomás H., Li Y.; Doxorubicin Loaded pH-sensitive Laponite/Alginate Nanohybrids: a Sustainable Release with Improved Anticancer Efficiency; 1st International Conference on Emerging Trends of Nanotechnology in Drug Discovery; New Delhi, India, 2014. (Invited oral presentation)
- MOCI.4. Rodrigues J., Castro R., Gonçalves M., Maciel D., Tomás H.; Dendrimers in Nanomedicine: A tool against older and emerging diseases?; 1st International Conference on Emerging Trends of Nanotechnology in Drug Discovery; New Delhi, India, 2014. (Keynote lecture)
- **MOCI.5.** Fernandes M. X., Martin-Higueras C., Salido E.; Searching for glycolate oxidase inhibitors in public chemical banks: leads for substrate reduction therapy in PH1; 11th International Primary Hyperoxaluria Workshop for Professionals, Patients and Families; Chicago, USA, 27-29 June, 2014.
- **MOCI.6.** Fernandes M. X.; Coupling phenotypic drug discovery and computational methods unravel anti-cancer therapeutic target; Chemical Approaches to Targeting Drug Resistance in Cancer Stem Cells, COST Action CM1106 2nd Workshop & CIBICAN Conference on Molecular Pharmacology and Mechanisms of New Anticancer Drugs, Puerto de la Cruz, Spain, October 14-15, 2014.
- **MOCI.7.** Fernandes M. X.; Reposicionamiento de fármacos: aplicación al caso de las enfermedades raras; XVIII Semana Científica Antonio Gonzalez Nuevas fronteras en Química Orgánica, La Laguna, Spain, October 6-10, 2014.



MOCI.8. Kong L., Hou W., Tomás H., Shi X.; RGD peptide-modified dendrimer-entrapped gold nanoparticles enable effective gene delivery to stem cells. Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014, POLY-614.

5.9.2 Invited seminars at other universities

- MIS.1. Rodrigues, J.; Huazhong University of Science and Technology, School of Chemistry and Chemical Engineering, (10 of April) Wuhan, P. R. China, **2014** (Invited speaker).
- MIS.2. Rodrigues, J.; Hubei University, College of Chemistry and Chemical Engineering, (10 of April), Wuhan, P. R. China, 2014 (Invited speaker).
- **MIS.3.** Rodrigues, J.; **Wuhan University**, College of Chemistry and Molecular Sciences (9 of April), Wuhan, P. R. China, **2014** (Invited speaker).
- MIS.4. Rodrigues, J.; Wuhan Textile University (WTU), School of Textile and Engineering (8 of April), Wuhan, P. R. China, 2014 (Invited speaker).
- MIS.5. Rodrigues, J.; Henan University of Technology, School of Chemistry and Chemical Engineering, (14 of Abril) Xinxiang, P. R. China, **2014** (Invited speaker).
- MIS.6. Rodrigues, J.; Zhengzhou University, College of Chymistry and Molecular Engineering, (15 of April), Zhengzhou, P. R. China, 2014 (Invited speaker).
- MIS.7. Rodrigues, J.; Henan Normal University (16 of April), Zhengzhou, P. R. China, **2014** (Invited speaker).
- **MIS.8.** Rodrigues, J.; **Donghua University**, College of Chemistry, Chemical Engineering, and Biotechnology, 17- 23 April, Shanghai, P. R. China, **2014** (Invited speaker).

5.9.3 Poster Communications

- **MPCI.1.** Araújo H., Pimenta A., Rivera I., Castro R., Tavares de Almeida I.; The impact of genetic factors and B-vitamin status on plasma homocysteine of portuguese children and adolescents; International Symposium of SPDM; 22-24 March 2014; Cascais, Portugal.
- **MPCI.2.** Araújo H., Pimenta A., Rivera I., Castro R., Tavares de Almeida I.; The one-carbon metabolism: evaluation of B-vitamin status and genetic factors on plasma homocysteine and methylmalonic acid levels in children and adolescent control groups; SSIEM Annual Symposium; 2-5 September 2014; Innsbruck, Austria.
- MPCI.3. Gonçalves M., Maciel D., Capelo D., Xiao S., Sun W., Shi X., Rodrigues J., Tomás H., Li Y.; Poly(amidoamine) dendrimer-mediated nanogels for drug delivery and intracellular tracking; 1st International Conference on Emerging Trends of Nanotechnology in Drug Discovery; New Delhi, India, 2014.

5.10 Abstracts in National Scientific Meetings

5.10.1 Oral Communications



- MOCN.1. Carla S. Alves, João Rodrigues, Helena Tomás, Yulin Li, Xiangyang Shi, Preparation of Dendrimer-Hyaluronic Acid Conjugate for Gold Nanoparticle Synthesis. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- **MOCN.2.** Nilsa Oliveira, João Rodrigues, Syntheses and Characterization of Novel Triazine Metallodendrimers. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.3. Dina Maciel, Mara Gonçalves, João Rodrigues, Helena Tomás, Yulin Li, Alginate/Laponite Hybrid Nanogels for Anticancer Drug Delivery. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.4. Carla Miguel, Nilsa Oliveira, Shili Xiao, João Rodrigues, Helena Tomás, Xiangyang Shi. Synthesis and Characterization of PEGylated Dendrimer-Entrapped Gold Nanoparticles. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.5. Manuel G. Jardim, João Rodrigues, José C. Mesquita, Kari Rinassen, Jochen Campo, Wim Wenseleers, Synthesis and Characterization of Novel Mix Metal Metallodendrimers for Nonlinear Optical Applications. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.6. Cláudia S. Camacho, João Rodrigues, Helena Tomás, Yulin Li, Folate-Functionalized PEGylated Low Generation PAMAM Dendrimers for Targeting Anticancer Drug Delivery. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.7. Kirthiga Ramalingam, Pedro Pires, Xiangyang Shi, João Rodrigues, Shili Xiao, Helena Tomás, Gene Delivery Using Dendrimer/pDNA Complexes Immobilized in Electrospun Nanofibers by the Layer-by-Layer (LbL) Technique. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.8. Diana M. Leite, J.M. Xavier, A. R. Ferreira, I. Amaral, Pedro L. Granja, Helena Tomás, A. P. Pêgo, Gene Therapy to the Central Nervous System: Exploring the Effect of Poly(amidoamine) (PAMAM)-NH2 Dendrimers on Neural Stem Cells. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- **MOCN.9.** Freddy Rodrigues, Miguel X. Fernandes, Design of Peptidomimetics Inhibitors. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.10. Guoying Wang, Dina Maciel, Xiangyang Shi, Yuan Yuan, Changsheng Liu, João Rodrigues, Helena Tomás, Yulin Li, Amphiphilic Polymer/Laponite Nanohybrids with Improved Stability and pH Sensitivity for Anticancer Drug Delivery. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.11. Mara Gonçalves, Dina Maciel, Débora Capelo, Shili Xiao, Wenjie Sun, Xiangyang Shi, João Rodrigues, Helena Tomás, Yulin Li, Alginate Nanogels Crosslinked with Calcium and Dendrimers for Drug Delivery and Intracellular Imaging. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.12. Akudari Raja Shekar, João Rodrigues, Helena Tomás, Yulin Li, Biodegradable Low Generation PAMAM Dendrimers for Drug Delivery. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.



- MOCN.13. Débora Capelo, Carla S. Alves, João Rodrigues, Helena Tomás, Yulin Li, PAMAM dendrimer/Hyaluronic Acid Nanoconjugates for Delivery of Doxorubicin . 1st
 CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.14. Xuedan He, Helena Tomás, Xiangyang Shi, RGD-modified Dendrimers for Drug Encapsulation and Targeted Inhibition of Tumor Angiogenesis. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.15. Neide Freitas, João Rodrigues, Nanotechnology: An Universe of Applications Impact on Cleaning Products. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.16. Rita Castro, Shili Xiao, Pedro L. Granja, João Rodrigues, Ana Paula Pêgo, Helena Tomás, New Materials Involving Self-assembly of Dendrimer-Chitosan-single Stranded DNA for Future Applications on Drug/gene Delivery. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.17. Inês J. Sousa, Rita Castro, João Rodrigues, Helena Tomás, Synthesis of Chitosan-PAMAM Dendrimer Nanoparticles. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.18. Andreia Pimenta, R. Castro, I. Tavares de Almeida, Helena Caldeira Araújo, S-Adenosylmethionine and Glucose-6-phosphate Activity in HUVEC cells. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.19. Miguel Xavier, Diana M. Leite, Pedro L. Granja, Helena Tomás, Ana Paula Pêgo, In-Vitro Modeling the Blood-Brain Barrier: A Tool for Assessing the Potential of PAMAM dendrimers as Vectors to the Central Nervous System. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- MOCN.20. Tiago Fernandes, João Rodrigues, Helena Tomás, Endocytosis Mechanisms of Dendrimers in Mesenchymal Stem Cells. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.

6. Organization of Conferences and Advanced Training Schools

The Nanoschool (advanced training school):

"Nanomedicines: Considerations for Design and Transfer into Clinical Use" (6-9 October **2014**). The lectures (8h) were presented by **Prof. Ruth Duncan** (Professor of Cell Biology and Drug Delivery, Professor Emerita, Cardiff University. U.K.); the school had around 40 participants.

7. INTERNATIONALIZATION

Beyond the national collaborations, the group has active collaborations (with joint publications/ongoing scientific work) with:

- Donghua University, College of Chemistry, Chemical Engineering and Biotechnology, China.
- Center for Advanced Research in Biotechnology, University of Maryland Biotechnology Institute, USA.



- Dep. of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, USA.
- Dep. of Organic Chemistry, Faculty of Chemistry, Vilnius University, Lithuania.
- Dep. de Química Física, Facultad de Química, Universidad de Murcia, Spain.
- Dep. de Física Fundamental y Experimental, Electrónica y Sistemas, Fac. de Física, Univ. of La Laguna, Spain.
- Dep. of Physical Chemistry, University of Oslo, Oslo, Norway.
- Dep. of Orthopaedics and Biochemistry & Molecular Genetics, University of Virginia, USA.
- Forschungszentrum Karlsruhe GmbH, Institut fur Nanotechnologie, Karlsruhe, Germany.
- Hubei University, Wuhan, China
- Instituto Canario de Investigación del Cáncer, Spain.
- Institut des Sciences Moléculaires, Univ. de Bordeaux I, France.
- Univ. of Antwerp, Belgium.
- NanoScience Center, Dep. of Chemistry, University of Jyväskylä, Finland.
- Nanotube Research Center, National Inst. of Advanced Industrial Science and Technology –AIST, Japan.
- Universidade Federal de Campina Grande, Centro de Ciências e Tecnologia, Brazil.
- Wuhan Textile University, Wuhan, China

In 2014, the level of internationalization of the Materials Group was also evidenced by the following:

- a) The group integrated several international networks (already mentioned);
- b) The group was organizer of a Nanoschool in the field of Nanochemistry and Nanomaterials (already mentioned);
- c) Prof. Xiangyang Shi is an Invited Full Professor at UMa (Chair in Nanotechnology, with the support of the Santander Bank and FCT) and also a researcher at Donghua University (China); the existence of this Chair in Nanotechnology is very important for CQM and, in particular, for the Materials Group, since it reinforced the knowledge in dendrimer chemistry at the group and, very importantly, allowed the exchange of students between CQM and Donghua University (since 2010, CQM regularly receives Chinese researchers for periods of training/research); furthermore, J. Rodrigues regularly visits Donghua University in 2014, he made a tour by several Chinese universities to discuss results of the ongoing research (especially at Donghua University), make seminars and exploit the possibility of additional collaborations with other professors in China;
- d) The group received two students from China for a period of research (Zhu Jingyi, PhD student, and Zhe Wang, a master student) in the scope of the Chair in Nanotechnology;



- e) Two Portuguese students (C. Miguel and C. Alves) went for a period of training/collaborative research to Donghua University (Shanghai, China) for 3 months;
- f) The group has PhD projects in collaboration with other international teams;
- g) H. Tomás was referee of research projects for the Polish National Science Center;
- h) The members of the group belong to several international professional societies and are referees of several journals with international circulation.



SCIENTIFIC REPORT OF THE NATURAL PRODUCTS GROUP I

1. GROUP DESCRIPTION

- Research Group Title: (RG-Madeira-674-391) Natural Products Group
- Principal Investigator: Paula Cristina Machado Ferreira Castilho
- Research Area: Natural Products
- Home Institution: Universidade da Madeira

2. Funding, source(s), dates

Available funding for 2014 | €499.862

Main Ongoing Projects and Grants headed by the Group:

FCT-IP funded:

- €600.000 (€150.000 for CQM): New-INDIGO/0003/2012. 2013-2016; PI: José
 Câmara (An attractive and promising strategy for early cancer diagnosis through
 the assembly of the Human Cancer Volatome)
- €166.696 (€114.860 for CQM): PTDC/CTM-CER/121295/2010. 2012-2015; PI: Paula Castilho (CLAYCATS4 Clay catalysts for biomass conversion)
- €69.553 (€30.502 for CQM): PTDC/AGR-ALI/122261/2010. 2012-2014; Participant: Paula Castilho (Desconstrução de Biomassa utilizando Super-ácidos Sólidos)
- €120.637 (€6.600 for CQM): PTDC/QUI-QUI/119116/2010. 2012-2015; Participant: Paula Castilho (Ocean Treasures Ocean sediments from Madeira Archipelago: a new source of innovative and bioactive compounds)
- € 47.040 (PhD grant): SFRH/BD/84672/2012. 2013-2017 (Vítor Spínola)
- €47.040 (PhD grant): SFRH/BD/97039/2013. 2014-2018 (Catarina Silva)
- € 53.820 (Post-Doc grant): SFRH/BPD/66177/2009. 2010-2015 (Jorge Pereira)
- € 53.820 (Post-Doc grant): SFRH/BPD/97387/2013. 2014-2017 (Rosa Perestrelo)

Projects and grants to be started in 2015:

Rubina Barros research grant from the Regional Delegation of the Portuguese League Against Cancer (Enderson Rodriguez)

3. OBJECTIVES AND ACHIEVEMENTS

3.1 Objectives

Global Scientific Report 2014



The goal of the natural products research group is the establishment of capabilities in the aspects of analysis, characterization and evaluation of core components of foodstuffs, and on the evaluation and identification of bioactive components of aromatic/medicinal plants, some of them also used as food constituents, on the search for new therapeutic molecules. The research is focused not only on the application but also on the development of techniques and methodologies of chemical analysis of volatile and non-volatile compounds in foodstuffs in order to characterize them and/or their processes of production and evolution. The same methods and techniques are being developed to establish chemotypes of botanical subspecies of Macaronesian biodiversity and to identify and quantify the essential oil and extract components with the aim of developing selected species into renewable sources of marketable products such as pharmaceuticals, biocides, fine chemicals, fuels, foods, and supplements. The same matrixes are characterized and evaluated for bioactive components, with relevance in food science and pharmacology. New matrixes, such as marine bacteria, are currently under study for the discovery and the isolation of new compounds with relevant biological/pharmaceutical properties. Furthermore, the group aims at building and maintaining a strong connection with the local institutions, by developing activity in the research and improvement of Madeira wine, a product of high economic importance, thus contributing to the development of the insular region where we live. The intertwining of expertise of the various members of the research group is actively procured in order to perform applied and fundamental research to achieve our objectives.

At the same time, the group is also developing new analytical methodologies that will allow an early diagnostic of several types of cancer through the analysis of the volatile compounds released from biological samples obtained using a non-invading process (like urine, breath, etc.).

3.2 Main Achievements

Through a reasonable number and size of projects that the members were able to secure during these years, the facilities and analytical park were much improved, leading to the attraction of national and international researchers and the training of existing collaborators.

At the end of 2014, the group consisted of 5 PhDs (2 members from the host institution, 1 from a State Laboratory and 2 Post-Doc researchers), 6 PhD students (5 FCT funded), 8 Master Students, and 5 researchers holding a Master's degree. The activity of the research group is demonstrated by the number of projects and the amount of funding obtained.

In 2014, the group published 10 papers in peer-reviewed journals with an average impact factor of 3.44⁴ and a degree of internationalization of 40%. Nine more papers were accepted for publication in international journals with impact factor, and 5 others have been submitted. Four book chapters, 3 papers in journals without impact factor, plus 2 Master Thesis were also published by team members of the Natural Products group. Additionally, 17 oral (9 in international conferences) and 30 poster communications (28 in international conferences) in scientific meetings were presented.

⁴Last impact factor available from year 2013. Global Scientific Report 2014



4. DISTINCTIONS, AWARDS AND MERITS

- Award for the best poster at the 1st Caparica Christmas Conference on Sample Treatment (8-10 December, 2014, Caparica, Portugal): Cavaco C.; Caldeira M.; Aveiro F., Pereira J.; Câmara J.S.; Characterization of potential volatile lung cancer biomarkers in saliva using solid phase microextraction followed by gas chromatography coupled to mass spectrometry, page 92, ISBN 978-989-98793-9-3.
- Paula Castilho is, since 2009, the representative member of the Area of Chemistry at the Scientific Board of the CCESE.

5. GROUP PRODUCTIVITY

5.1 Published Articles in Peer-Reviewed Journals (IF)

- **P.1.** Figueira J.; Câmara H.; Pereira J.; Câmara J. S.; Evaluation of volatile metabolites as markers in Lycopersicon esculentum L. cultivars discrimination by multivariate analysis of headspace solid phase microextraction and mass spectrometry data; *Food Chem.* 2014, 145, 653-663; DOI: 10.1016/j.foodchem.2013.08.061 (IF: 3.259).
- **P.2.** Gonçalves J.L.; Figueira J.A.; Rodrigues F.P.; Branco B.; Câmara J.S.; A powerful methodological approach combining headspace solid phase microextraction, mass spectrometry and multivariate analysis for profiling the volatile metabolomic pattern of beer starting raw-materials. *Food Chem.* 2014, 160, 266-280; DOI: 10.1016/j.foodchem.2014.03.065 (IF: 3.259).
- **P.3.** Pereira J.; Câmara J. S.; Colmsjö A.; Abdel-Rehim M.; Microextraction by packed sorbent: an emerging, selective and high-throughput extraction technique in bioanalysis; *Biomed. Chromatogr.* 2014, 28, 839-847; DOI: 10.1002/bmc.3156 (IF: 1.662).
- **P.4.** Pereira J.; Silva C. L.; Perestrelo R.; Goncalves J.; Alves V.; Camara J. S.; Re-exploring the high-throughput potential of microextraction techniques, SPME and MEPS, as powerful strategies for medical diagnostic purposes. Innovative approaches, recent applications and future trends; *Anal. Bioanal. Chem.* 2014, 406, 2101-2122; DOI: 10.1007/s00216-013-7527-4 (IF: 3.578).
- P.5. Qiao Z.; Perestrelo R.; Shi X.; Rodrigues J.; Câmara J.S.; An exploratory study to evaluate the potential of nanohydroxyapatite as a powerful sorbent for efficient extraction of volatile organic metabolites, potential biomarkers of cancer, *Anal. Methods* 2014, 6, 6051-6057; DOI: 10.1039/C4AY00997E (IF: 1.938).
- P.6. Perestrelo R.; Silva C.L.; Câmara J.S.; Gas chromatography combined with mass spectrometry data as useful approach for wines differentiation according to geographical origin based on global volatile patterns, J. Sep. Sci. 2014, 37, 1974-1981; DOI: 10.1002/jssc.201400374 (IF: 2.594).
- **P.7.** Perestrelo R.; Barros A.S.; Rocha S.M.; Câmara J.S.; Establishment of Vitis vinifera L. grape varieties varietal profile from different geographical regions based on HS-



- SPME/GC-qMS combined with chemometric tools, *Microchem. J.* 2014, 16, 107-117; DOI: 10.1016/j.microc.2014.04.010 (IF: 3.583).
- P.8. Castilho P.; Vilcocq L.; Carvalheiro F.; Duarte L. C.; Hydrolysis of oligosaccharides over solid acid catalysts a review *ChemSusChem* 2014, 7, 1010 1019; DOI: 10.1002/cssc.201300720 (IF: 7.117).
- **P.9.** Spínola V.; Llorent-Martínez E.J.; Gouveia S.C.; Castilho P.C.; Myrica faya: a new source of antioxidant phytochemicals; *J. Agric. Food Chem.*, 2014, *62* (40), 9722–9735; DOI: 10.1021/jf503540s (IF: 3.107).
- **P.10.** Spínola V.; Llorent-Martínez E.J.; Castilho P.C.; Determination of vitamin C in foods: current state of method validation; *J. Chromatogr. A,* 2014, 1369, 2-17; DOI:10.1016/j.chroma.2014.09.087 (IF: 4.258).

5.2 Book Chapters

- **PBC.1.** Câmara J.S.; Figueira J., Perestrelo R.; Silva C.L.; Pereira J.; Bioactive Compounds from Different Food Sources: Biosynthesis, Occurrence and Potential Health Benefits. In: Biochemistry Research Trends. Editor Dean T. Cobb. Nova Science Publishers Inc. 2014. ISBN: 978-1-63117-858-0.
- PBC.2. Gouveia S. C.; Spínola V.; Castilho P. C.; Chapter 1: Phenolic Compounds and Antioxidant Capacity of Medicinal Plants: A Review. In: Medicinal Plants: Antioxidant Properties, Traditional Uses and Conservation Strategies, pages 1-41, Publisher: Nova Science Publishers, Inc. 09/2013; 2014; ISBN: 978-1-62948-220-0 (eBook).
- PBC.3. Perestrelo R.; Silva C.L.; Pereira J.; Câmara J.S.; Healthy Effects of Bioactive Metabolites from *Vitis vinifera* L. Grapes: A Review. In: Grapes: Production, Phenolic Composition and Potential Biomedical Effects. Editors: José de Sousa Câmara. Food and Beverage Consumption and Health Series. Nova Science Publishers Inc. 2014. Chap. 13, ISBN: 978-1-63321-410-1.
- **PBC.4.** Perestrelo R.; Silva C.L.; Pereira J.; Câmara J.S.; Madeira, Port and sherry fortified wines: the *sui generis* and notable peculiarities, major differences and chemical patterns, Part II, Encyclopedia of Food and Health, Elsevier, London, 2014.

5.3 Published Papers in International Journals With Peer Review But Without Impact Factor

- **PPWF.1.** Cavaco C.; Perestrelo R.; Silva C. L.; Aveiro F.; Pereira J.; Câmara J.S. Establishment of the Saliva Volatomic Profile as an Exploratory and Non-invasive Strategy to Find Potential Breast Cancer Biomarkers. *Int. Labmate*. 2014, 68-69.
- **PPWF.2.** Silva C.; Cavaco C.; Perestrelo R.; Pereira J.; Câmara J.S.; Microextraction by Packed Sorbent (MEPS) and Solid-Phase Microextraction (SPME) as Sample Preparation Procedures for the Metabolomic Profiling of Urine; *Metabolites* 2014, 4, 71-97.(*New journal*)



PPWF.3. Gouveia-Figueira S.C., Gouveia C.A.; Carvalho M.J.; Rodrigues A.I., Nording M.L., Castilho P.C.; Antioxidant Capacity, Cytotoxicity and Antimycobacterial Activity of Madeira Archipelago Endemic *Helichrysum* Dietary and Medicinal Plants. *Antioxidants*. 2014, 3, 713-729. DOI: 10.3390/antiox3040713. (New journal)

5.4 Accepted Papers in International Journals

- **PAP.1.** Catrinescu C.; Fernandes C.; Castilho P.; Breen C.; Selective methoxylation of α -pinene to α -terpinyl methyl ether over Al3+ ion-exchanged clays; *Appl. Catal. A: Gen.*, 2015, 489, 171-179; DOI: 10.1016/j.apcata.2014.10.028. (IF: 3.674).
- **PAP.2.** Spínola V.; Perestrelo R.; Câmara J.S.; Castilho P.C.; Establishment of Monstera deliciosa fruit volatile metabolomic profile at different ripening stages using solid-phase microextraction combined with gas chromatography–mass spectrometry, *Food Res. Int.*, 2015, 67, 409-417; DOI:10.1016/j.foodres.2014.11.055 (IF: 3.05)
- **PAP.3.** Fernandes P.; Barros N.; Santo J.L.; Câmara J.S.; Evaluation of the co-occurring mycotoxins in cereals by a modified QuEChERS extraction procedure and dispersive solid extraction clean-up combined with liquid chromatography—triple quadrupole tandem mass spectrometry. *Food Anal. Met., 2015*; DOI: 10.1007/s12161-014-9947-y (IF: 1.802).
- PAP.4. Pereira J.; Porto-Figueira P.; Cavaco C.; Taunk K.; Rapole S.; Dhakne R.; Nagarajaram H.; Câmara J.; Breath analysis as a potential and non-invasive frontier in disease diagnosis. A metabolomic approach. *Metabolites*; DOI: 10.3390/metabo5010003 (IF: 2.500).
- **PAP.5.** Perestrelo R.; Silva C.L.; Câmara J.S.; Quantification of furanic derivatives in fortified wines by a highly sensitive and ultrafast analytical strategy based on digitally controlled microextraction by packed sorbent combined with ultrahigh pressure liquid chromatography. *J. Chromatogr. A*, 2015; DOI: 10.1016/j.chroma.2015.01.020 (IF: 4.308).
- **PAP.6.** Qiao Z.; Perestrelo R.; Reyes-Gallardo E.M.; Lucena R, Cardenas M.; Rodrigues J.; Câmara J.S.; Octadecyl functionalized core-shell magnetic silica nanoparticle as a powerful nanocomposite sorbent to extract urinary volatile organic metabolites. *J. Chromatogr. A*, 2015; DOI: 10.1016/j.chroma.2015.03.026 (IF: 4.308).
- PAP.7. Spínola V.; Pinto J.; Castilho P.C.; HPLC-DAD-ESI-MSn screening of phenolic compounds and antioxidant activity of selected fruits from Madeira island. *Food Chem.*, 2015, 173, 14-30; DOI: 10.1016/j.foodchem.2014.09.163 (IF: 3.259).
- **PAP.8.** Llorent-Martínez E.J.; Gouveia S.C.; Castilho P.C.; Analysis of phenolic compounds in leaves from endemic trees from Madeira Island. A contribution to the chemotaxonomy of Laurisilva forest species. *Ind. Crop Prod.* 2015, 64, 135–151; DOI 10:1016/j.indcrop.2014.10.068 (IF: 3.208).
- **PAP.9.** Catrinescu C.; Fernandes C.; Castilho P.C.; Breen C.; Selective methoxylation of α -pinene to α -terpinyl methyl ether over Al3+ ion-exchanged clays. *Appl. Catal. A: Gen.*, 2015, 489, 171-179; DOI: 10.1016/j.apcata.2014.10.028 (IF: 3.674).



5.5 Thesis

- **PTH.1.** Joana Pereira; Produção de Monoglicéridos Através de Catalisadores de Argila. Thesis presented to obtain the Master degree, Universidade da Madeira, 2014. Supervisor: Paula Castilho, co-supervisor: César Fernandes.
- **PTH.2.** Zheng Qiao; Evaluation of the sorbent properties of carbon nanotubes and related nanosctuctures as a basis to develop a nanotrap device to isolate the volatiles metabolites from biologic fluids. Thesis presented to obtain the Master degree, Universidade da Madeira, 2014. Supervisor: José Câmara, co-supervisor: João Rodrigues.

5.6 Abstracts in International Scientific Meetings

5.6.1 Oral Communications

- **POCI.1.** Câmara J.S. An attractive and promising strategy for early cancer diagnosis through the assembly of the Human Cancer Volatome. Human Cancer Metabolome (HCV) project meeting, 29th-31st January 2014, Rostock, Germany. (**invited oral presentation**)
- **POCI.2.** Perestrelo R., Rodrigues J., Câmara J.S.; Mass spectrometry in Dendrimers characterization: analytical overview; 1st International Conference on Emerging Trends of Nanotechnology in Drug Discovery; New Delhi, India; 26-27 May, page 6, 2014. (invited oral presentation)
- **POCI.3.** Porto-Figueira P., Câmara J.S. Exploring the potentialities of a new and high-throughput ultrasound-assisted μ-QuEChERS-based extraction technique combined with UHPLC-FLR, for determination of Zearelenone in cereals. 16th International Symposium on Advances in Extraction Technologies. ExTech 2014, Crete, Greece; 25-28 May 2014.
- **POCI.4.** Perestrelo R., Silva C.L., Câmara J.S. Establishment of furanic derivatives fingerprint of fortified wines through a new and ultrafast analytical approach based on digitally controlled MEPS extraction combined with RP-UHPLC. 30th International Symposium on chromatography. ISC2014. Salzburg, Austria. 14-18 September 2014.
- **POCI.5.** Silva C.L., Perestrelo R., Câmara J.S. An improved and highly sensitive procedure based on microextraction by packed sorbent (MEPS) combined with ultrahigh pressure liquid chromatography for quantification the urinary levels of leukotriene B4. Garda, Italy, May, page, 2014.
- **POCI.6.** Porto-Figueira P., Figueira J.A., Pereira J., Câmara J.S., "Evaluation of the efficiency of an innovative extraction technique, SPEed, for the analysis of free lowmolecular weight polyphenols in different food matrices", XX Encontro Luso Galego de Química, 26 a 28 de Novembro de 2014, Complexo FFUP/ICBAS, Porto. ISBN 978-989-98541-7-8, pag. 275.
- **POCI.7.** Figueira J.A., Porto-Figueira P., Câmara J.S., "Determination of lipophilic antioxidants, δ and α tocopherol, in Lycopersicon esculentum L. from gordal variety at maturity, by LL-USAE/UHPLC-FLR", XX Encontro Luso Galego de Química,



- 26 a 28 de Novembro de 2014, Complexo FFUP/ICBAS, Porto. ISBN 978-989-98541-7-8.
- **POCI.8.** Castilho P.C., Vilcocq L., Duarte L.C., Carvalheiro F., Fernandes C.; Solid Acid Catalysts for the Hydrolysis of Oligossacharides Frontiers in Biorefining International Conference, St. Simons Island, Georgia, USA 21-24 October 2014
- **POCI.9.** Branco, P.C.; Torrado, I.; Dionísio, A.M.; Carvalheiro, F.; Duarte, L.C.; Castilho, P.C., Wastes from agro-food industries as raw materials for the production of biofuels and bioproducts, Seminar on Renewable Energies and Environment, Portalegre, Portugal, May 2014.

5.6.2 Poster Communications

- **PPCI.1.** Cavaco C.; Caldeira M.; Aveiro F., Pereira J.; Câmara J.S.; Characterization of potential volatile lung cancer biomarkers in saliva using solid phase microextraction followed by gas chromatography coupled to mass spectrometry. 1st Caparica Christmas Conference on Sample Treatment, 8th, 9th, 10th of December, 2014, Caparica, Portugal, page 92, ISBN 978-989-98793-9-3 awarded with the best poster distinction.
- **PPCI.2.** Porto-Figueira P; Figueira J; Pereira J; Câmara J.S.; SPEed, an innovative extraction technique for the quantification of free low-molecular weight polyphenols in tea and wines. 1st Caparica Christmas Conference on Sample Treatment, 8th, 9th, 10th of December, 2014, Caparica, Portugal, , page 91, ISBN 978-989-98793-9-3
- **PPCI.3.** Rodriguez E., Pedro P., Castillo M., Perestrelo R., Câmara J.S.; Simulating the formation of furanic derivatives in wines using Synthetic Model Wines and HS-SPME/GC-qMS, XX Encontro Luso-Galego de Química, Porto, Portugal, 26-28 November, page 291, 2014.
- **PPCI.4.** Pedro P., Rodriguez E., Castillo M., Perestrelo R., Câmara J.S.; Evaluation of storage temperature and time on furanic derivates formation by MEPS/UHPLC-PDA, XX Encontro Luso-Galego de Química, Porto, Portugal, 26-28 November, page 292, 2014.
- **PPCI.5.** Castillo M., Rodriguez E., Perestrelo R., Câmara J.S.; HS-SPME/GC-qMS como poderosa estratégia analítica na avaliação da influência de diferentes processos de vinificação no perfil volátil de vinhos Madeira, XX Encontro Luso-Galego de Química, Porto, Portugal, 26-28 November, page 287, 2014.
- **PPCI.6.** Cavaco C.; Caldeira;; Aveiro F.; Pereira J.; Câmara J.S.; A noninvasive sampling procedure combined with a powerful analytical strategy and multivariate analysis for detection of volatile metabolites potential lung cancer biomarkers. XX Encontro Luso-Galego de Química, Porto, Portugal, 26-28 November, 2014
- **PPCI.7.** Alves V.; Gonçalves J.; Teixeira H.; Câmara J.S. A powerful strategy based on microextraction by packed sorbent combined with UHPLC-PDA for simultaneous analysis of fluoxetine and clomipramine and their active metabolites in human urine. XX Encontro Luso-Galego de Química, Porto, Portugal, 26-28 November, 2014.



- **PPCI.8.** Spínola V., Perestrelo R., Câmara J., Castilho P. Profiling of volatiles in fruits of Monstera deliciosa based on headspace solid phase microextraction and mass spectrometry analysis, 30th International Symposium on Chromatography, Salzburg, Austria, 14-18 September, page 85, 2014.
- **PPCI.9.** Perestrelo R., Qiao Z., Reyes-Gallardo E., Lucena R., Rodrigues J., Cárdenas S., Câmara J.S.; Evaluation of the efficiency of a surface hydrophobic carbon-ferromagnetic nanocomposite on urinary volatile organic metabolites extraction, 30th International Symposium on Chromatography, Salzburg, Austria, 14-18 September, page 97, 2014.
- **PPCI.10.** Silva C.L.; Aveiro F.; Câmara J.S.; Non-invasive, innovative and promising strategy for early diagnosis of breast cancer based on urinary volatile metabolites. 30th International Symposium on Chromatography, Salzburg, Austria, 14-18 September, page 97, 2014.
- **PPCI.11.** Cavaco C.; Silva C.L.; Perestrelo R.; Aveiro F.; Pereira J.; Câmara J.S.; Establishment of the saliva volatomic profile as an exploratory and non-invasive strategy to find potential breast cancer biomarkers; 38th International Symposium on Capillary Chromatography and 11th GCxGC Symposium, Riva del Garda, Italy, May, page 480, 2014.
- PPCI.12. Câmara J.S.; Perestrelo R.; Silva C.L.; An unexplored strategy based on semiautomatic MEPS procedure followed by UHPLC-PDA as an highly sensitive and specific methodology to quantify the urinary levels of leukotriene B4; 38th International Symposium on Capillary Chromatography and 11th GCxGC Symposium, Riva del Garda, Italy, May, page 476, 2014.
- **PPCI.13.** Ideia P., Pinto J.; Morna A.; Pereira J.; Camara J.S.; Metabolite profiling on coffee volatile composition based on solid phase microextraction and gaschromatography quadrupole mass spectrometry. 38th International Symposium on Capillary Chromatography and 11th GCxGC Symposium, 18-23 May 2014, Riva del Garda, Italy. page eee, 2014
- **PPCI.14.** Cavaco, C.; Silva, C.L.; Perestrelo, R.; Aveiro, F.; Jorge Pereira, J.; Câmara, J.S.; Establishment of the saliva volatomic profile as an exploratory and non-invasive strategy to find potential breast cancer biomarkers; 38th International Symposium on Capillary Chromatography and 11th GCxGC Symposium, Riva del Garda, Italy, May, page 480, 2014.
- PPCI.15. Câmara, J.S.; Perestrelo, R.; Silva, C.L.; An unexplored strategy based on semiautomatic MEPS procedure followed by UHPLC-PDA as an highly sensitive and specific methodology to quantify the urinary levels of leukotriene B4; 38th International Symposium on Capillary Chromatography and 11th GCxGC Symposium, Riva del Garda, Italy, May, page 476, 2014.
- **PPCI.16.** Porto-Figueira, P; Figueira, J.A.; Câmara, J.S.; Headspace solid phase microextraction tandem with gas chromatography-mass spectrometry analysis as useful strategy to establish the volatomic profile of blackberry fruit. 38th International Symposium of Capillary Chromatography and 11th GC x GC Symposium, Riva del Garda, Italy, May, page 532, 2014.



- **PPCI.17.** Porto-Figueira, P.; Freitas A.; Cruz C.; Figueira, J.A.; Câmara, J.S. Screening of the volatomic profile of different Passiflora L. species through headspace solid phase microextraction tandem with gas chromatography-mass spectrometry analysis. 38th International Symposium of Capillary Chromatography and 11th GC x GC Symposium, Riva del Garda, Italy, May, page 520, 2014.
- **PPCI.18.** Porto-Figueira, P; Figueira, J.A.; Câmara, J.S.; Comparison of the effectiveness of different extraction techniques, spme and quechers, combined with gas chromatography—mass spectrometry for the establishment of the volatomic profile of Eugenia uniflora L.. 38th International Symposium of Capillary Chromatography and 11th GC x GC Symposium, Riva del Garda, Italy, May, page 219, 2014.
- **PPCI.19.** Alves V.; Gonçalves J.; Teixeira M.H.; Camara J. S. Simultaneous quantification of fluoxetine, clomipramine and their active metabolites in human urine samples based on microextraction by packed sorbent followed by UHPLC-PDA analysis. 38th International Symposium on Capillary Chromatography and 11th GCxGC Symposium, Riva del Garda, Italy, May, 2014.
- PPCI.20. Gonçalves L.; Alves V., Teixeira M.H.; Camara J. S. A powerful strategy based on microextraction by packed sorbent combined with UHPLC-PDA for analysis of risperidone, clozapine and their active metabolites in human urine. 38th International Symposium on Capillary Chromatography and 11th GCxGC Symposium, Riva del Garda, Italy, May, 2014.
- **PPCI.21.** Porto-Figueira, P; Figueira, J.A.; Câmara, J.S.; Exploring the potentialities of a new and high-throughput ultrasound-assisted μ-QuEChERS-based extraction technique combined with UHPLC-FLR, for determination of Zearelenone in cereals; ExTech 2014, 16th International Symposium on Advances in Extraction Technologies, Chania, Crete, Greece, May, page 53, 2014.
- PPCI.22. Mendes B.; Pereira J.; Câmara J.S.; An improved and fast methodology based on eVol-MEPS/UHPLC-PDA analysis to assess the urinary profile levels of oxidative damage biomarkers in cardiovascular diseases risk development. ExTech 2014, 16th International Symposium on Advances in Extraction Technologies, Chania, Crete, Greece, 25th-28th May 2014.
- **PPCI.23.** Qiao, Z.; Perestrelo, R.; Shi, X.; Rodrigues, J.; Câmara, J.S.; Nanohydroxyapatite as a new nanomaterial for efficient extraction of volatile metabolites viewed as potential biomarkers of cancer; ExTech 2014, 16th International Symposium on Advances in Extraction Technologies, Chania, Crete, Greece, May, page 89, 2014.
- **PPCI.24.** Perestrelo, R.; Silva, C.L.; Câmara, J.S.; A new, reliable and high throughput analytical approach for the simultaneous determination of furans in wine matrices; ExTech 2014, 16th International Symposium on Advances in Extraction Technologies, Chania, Crete, Greece, May, page 135, 2014.
- **PPCI.25.** Castilho P.C., Catrinescu C., Fernandes C., Breen C.; Methoxylation of a-pinene over ion exchanged clays Frontiers in Biorefining International Conference, St. Simons Island, Georgia, USA 21-24 October 2014.
- **PPCI.26.** Dionisio A.M., Branco P.C., Torrado I., Roseiro L.B., Carvalheiro F., Castilho P.C., Duarte L.C.; Oligosaccharides production from Anonna cherimola Mill. seeds:



- optimization and modelling ChemPor 2014, Porto, Portugal September 2014, poster P-CM19.
- **PPCI.27.** Spínola, V., Perestrelo R., Câmara, J.S., Castilho P.C. Profiling of volatiles in fruits of Monstera deliciosa based on headspace solid phase microextraction and mass spectrometry analysis, 30th International Symposium on Chromatography, 14 18 September 2014 Salzburg, Austria. Poster P266-SF-TU.
- **PPCI.28.** Spínola V., Llorent-Martínez E.J., Gouveia S.G., Castilho P.C.; Myrica faya: phenolic characterization and antioxidant activity, Polyphenols, 4-6 June, Lisbon, Portugal, 2014, poster 156.

5.7 Abstracts in National Scientific Meetings

5.7.1 Oral Communications

- OCN.1. Catarina L. Silva, Rosa Perestrelo, José S. Câmara, An Improved and Highly Sensitive Procedure Based on Microextraction by Packed Sorbent (MEPS) Combined with Ultra High Pressure Liquid Chromatography for Quantification of Urinary Levels of Leukotriene B4. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- **OCN.2.** Vítor Spínola, Eulogio J. Llorent-Martínez, Sandra Gouveia, Paula C. Castilho, Phenolic Composition of Myrica faya and its Relation with Antioxidant Activity. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- **OCN.3.** Vítor Spínola, Milangela Heyden, Paula C. Castilho, Simultaneous Chromatographic Quantification of Oxalic and L-ascorbic Acids in Foodstuffs. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- **OCN.4.** Maria Fátima Sousa, José S. Câmara, Luis Dantas, Rita Vasconcelos, Maria Natália Silva, Dora Aguin-Pombo, Volatile Composition and Behavioral Responses of Ceratitis capitata (Diptera: Tephritidae) to Five Native and Exotic Plants of Madeira. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- **OCN.5.** Carina Cavaco, Jorge Pereira, Fernando Aveiro, José S. Câmara, Establishment of the metabolomic volatile profile of urine and saliva, as powerful and non-invasive strategy, for the detection of potential biomarkers of different types of cancer. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- **OCN.6.** Eulogio J. Llorent-Martínez, Sandra Gouveia, Vítor Spínola, Paula C. Castilho, Mass Spectrometry for the Determination of Species of Interest in Plants and Plantderived Foods. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- OCN.7. José A. Figueira, José S. Câmara, Determination of Lipophilic and Hydrophilic Antioxidants in Tomato of Lycopersicon esculentum L., Gordal Variety at Different Growth Stages. Correlation with Antioxidant Capacity. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.
- **OCN.8.** Joana Pereira, César Fernandes, Paula C. Castilho, Preparation of Monoglycerides by Heterogeneous Catalysis. 1st CQM Annual Meeting. 31st January-1st February 2014, Funchal, Madeira.



5.7.2 Poster Communications

- **PPCN.1.** Porto-Figueira P; Freitas A.; Cruz C.; Figueira J; Câmara J.S.; Differentiation of the volatomic pattern of several Passiflora L. species. XII Encontro de Química dos Alimentos, 9-12 September, 2014, Lisbon.
- **PPCN.2.** Porto-Figueira P; Figueira J; Câmara J.S.; Development of a new and high-throughput ultrasound-assisted μ-QuEChERS-based extraction technique combined with UHPLC-FLR for determination of Zearalenone in cereals. XII Encontro de Química dos Alimentos, 9-12 September, 2014, Lisbon.

5.8.3 PATENTS

- **PPT.1.** Duarte, L.C., **Branco, P.C.,** Torrado, I., Klydjeneiro, Z., Pereira, C., Roseiro, L., Roseiro, J.C., **Castilho, P.C.**, Carvalheiro, F. (**2013**). Patent pending: PT 106355
- **PPT.2.** Duarte, L.C., **Branco, P.C.**, Torrado, I., Klydjeneiro, Z., Pereira, C., Roseiro, L., Roseiro, J.C., **Castilho, P.C.**, Carvalheiro, F. (**2013**). Patent pending: PT 106354
- **PPT.3.** Duarte, L.C., **Branco, P.C.,** Torrado, I., Klydjeneiro, Z., Pereira, C., Roseiro, L., Roseiro, J.C., **Castilho, P.C.**, Carvalheiro, F. (**2013**). Patent pending: PT 106353

6. ORGANIZATION OF CONFERENCES

 2nd Meeting of the project HCV - "An attractive and promising strategy for early cancer diagnosis through the assembly of the Human Cancer Volatome" (New-INDIGO/0003/2012), funded by European Funds (New INDIGO Partnership Programme, co-funded by FP7.

7. Internationalization

Although 2014 publications showed predominantly results of national collaborations (the degree of internationalization was 40%), international cooperation was actively pursued. Some previously established collaborations with the Instituto Canario de Investigacion en Cancer, the Institute of Tuberculosis Research, University of Chicago Illinois and the Instituto Politecnico Nacional of Mexico, were of key importance for the ongoing research programs on the isolation, characterization and evaluation of metabolites of plant origin, with special incidence on those with antitumor and antituberculosis activity. New projects will bring new partnerships with international institutions such as the prestigious Scripps Institution of Oceanography - University of California San Diego (SIO-UCSD). This institute is a partner in the project "Ocean Treasures" which aims to explore the active metabolites produced by deep sea bacteria from Madeira Island. Old partnerships are being revived. Back in 2000, collaboration with the Materials and Engineering Research Institute (MERI) from Sheffield Hallam University, UK, was established in the form of the CLAYCATS project for the production and

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characterization of clay-based catalysts. This collaboration is now re-opened in the form of the CLAYCATS4 project, a more focused project on the application of catalysts on biomass conversion and bioactive molecules hemisynthesis.

In addition, a large Indo-European consortium is involved in the project (Indigo Project) headed by J.S. Câmara (An attractive and promising strategy for early cancer diagnosis through the assembly of the Human Cancer Volatomics). The partners involved are: INDIA: National Center for Cell Science (NCCS), Ganeshkhind, Pune (Indian Coordinator, Prof. Rapole Shrikanth) and Centre for DNA Fingerprinting & Diagnostics (CDFD) Bldg7, Gruhakalpa, Nampally (Prof. Hampapathalu Nagarajaram); GERMANY: University of Rostock, Faculty of Medicine (Prof. Jochen Klaus Schubert).

The group received an Erasmus visitant - Professor Cezar Catrinescu from Iasi University, Romania, 9-23 September 2014. Also, the student Felix Mueller worked in the group (Student internship, in Internship from Eberswalde University of Sustainable Development Faculty of Forest and Environment, September 2014-February 2015).



CQM FACTS AND FIGURES

1. HUMAN RESOURCES

THE RESEARCH TEAM OF CQM (M-MALE, F-FEMALE) IS COMPOSED OF THE FOLLOWING:

CQM research staff (31 of December 2014)	M(%)	F(%)	Total
Ph Ds	9	6	15
Ph D Students	6	5	11
Co-workers	3	6	9
Researchers with a Master degree	4	5	9
Master Students	6	7	13
Other co-workers	-	-	-
TOTAL	28(50)	29 (51)	57

(QUADRO RESEARCH TEAM)

Only 57% of CQM team members are full time researchers. The remaining 43% are also involved in research, administrative, teaching and other activities. At the end of 2014, the research team average age was 33 years, 15% were expatriates (mainly from People's Republic of China) and 51% were women.

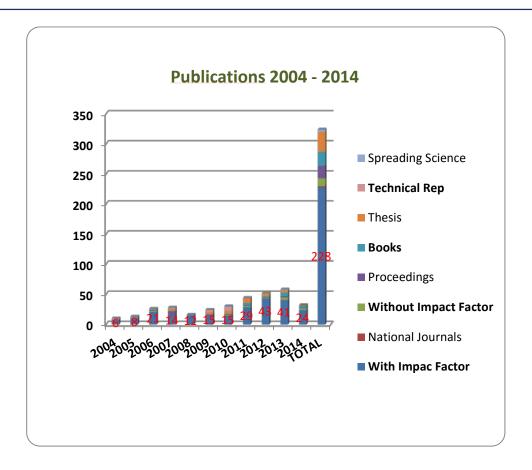
2. BUDGET 2004-2016

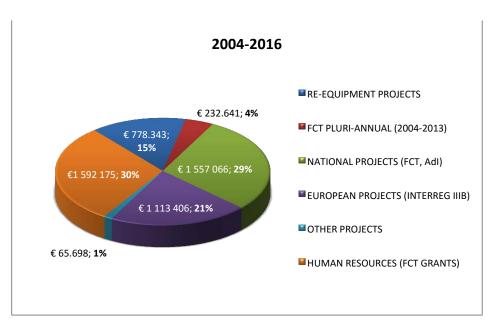
In the period 2011-2014, CQM managed a total of \leqslant 3 216.585, including a total of approved funds in the same period of \leqslant 1 582.563. This amount, together with previously funded projects supported by different entities (*e.g.* FCT, INTERREG IIIB), sum-up more than \leqslant 5.3 million in the period 2004-2016.

3. PUBLICATIONS 2004-2014

At the end of 2014, the CQM had around 345 publications, including 228 with impact factor (113 published in the period 2011-2014).





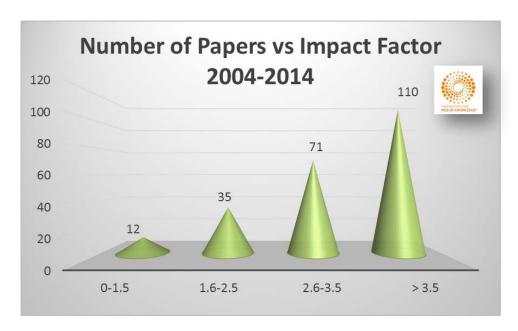


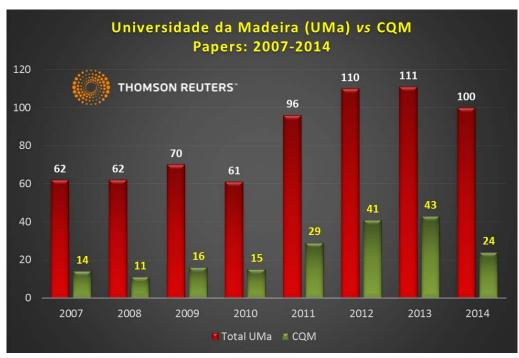
In the 2004-2016 periods the direct and indirect FCT support reached the total amount of €4.1 million (ca. 78% of the total available budget).



Impact Factor

• The distribution of the number of CQM publications *versus* the impact factor, in the period 2004-2014, shows that in an total of 228 papers published with IF, 48% has an impact factor greater than 3.5, 11 papers has IF higher than 8 and 1 with IF higher than 24.



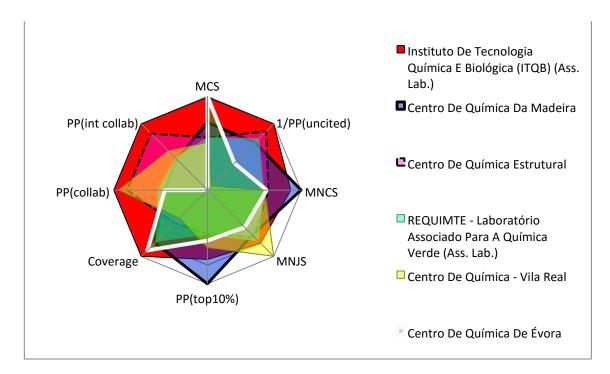




4. CQM BIBLIOMETRIC RESULTS 2007- 2010

The Foundation for Science and Technology (FCT-IP) recently published the results of a commissioned bibliometric study from the Center for Science and Technology Studies (CWTS) of the University of Leiden (http://bit.ly/1c7cf6L). The principal aim of this study was to map the scientific contributions of the Research Units and Associated Laboratories supported by the pluriannual funding program of FCT-IP. The study examined all publications of each of the funded institutions that are registered on the WoS – Web of Science between the years 2007 and 2010, and produced a set of indicators to compare and assess the quality of scientific output.

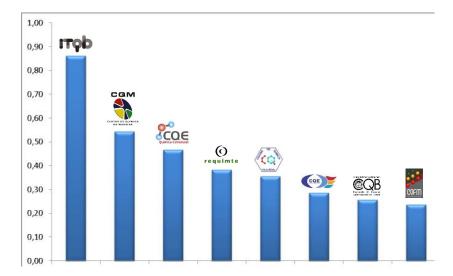
The statistical analysis of bibliometric indicators shows that, in the considered period, the Centro de Química da Madeira (CQM) reached an excellent standard of quality, achieving the highest score in two (MNCS & PP(top 10%)) of the eight indicators (see next graph).



Graph: Statistical analysis of bibliometric indicators for the chemistry area: PP (top10%) – Percentage of highly cited publications; MNCS – Mean field normalized citation score (The full list of abbreviations and related details is available in page 76 of this report).

Considering all indicators, and comparing with all Portuguese institutions that conducted research in the field of Chemistry (15), the CQM lies the in the second place (see next graph). This result is especially important given that from the first four institutions, the CQM is the only one with less than a hundred researchers.





Graph: Score of the first eight portuguese institutions that conduct research in the field of Chemistry in Portugal (Data based in publications from 2007-2010; WoS – Web of Science).

Abbreviations list used in the study (From FCT-IP web site):

- P Number of publications in international journals of the unit of analysis in the entire period;
 - MCS Average number of citations without self citations per paper;
- PP (uncited) Percentage of publications not cited by others (in the given time period);
- MNCS Mean field normalized citation score. This is the actual number of citations (without self-citations) divided by the expected number of citations on a paper basis. The expected number of citations is based on the world-wide average citation score without self-citations of all similar papers belonging to the same field (journal subject category). In this way, a field normalized score is calculated for each paper. Next, the MNCS indicator is computed for the unit of analysis by taking the average of these field-normalized citation scores for individual papers. A value above 1 indicates that the mean impact for the unit is above world average whereas a value below 1 indicates the opposite.
- MNJS Mean normalized journal score. Indicates the average citation impact of the journals that are used by the unit and is calculated based on the same principles as the MNCS. The indicator shows whether the unit publishes in top or in sub-top journals.
- PP (top10%) Percentage of highly cited publications. Indicates the average citation impact of the journals that are used by the unit and is calculated based on the same principles as the MNCS. The indicator shows whether the unit publishes in top or in sub-top journals.
- Coverage Internal coverage. Measured by the proportion of cited references in the oeuvre linking to other WoS publications;
- PP (collab) Publications that are done in institutional collaboration (the shares are calculated based on the total number of publications);



• PP (int collab) – Publications that are perfomed among institutions of more than one country (the shares are calculated based on the total number of publications);

"no collaboration" - Publications from a single FCT institute;

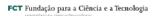
"national collaboration" - Publications from at least two authors in the same country (Portugal);

"international collaboration" - Publication from FCT funded institutes with one or more foreign (non-Portuguese) institutions.



ACKNOWLEDGMENTS I

















































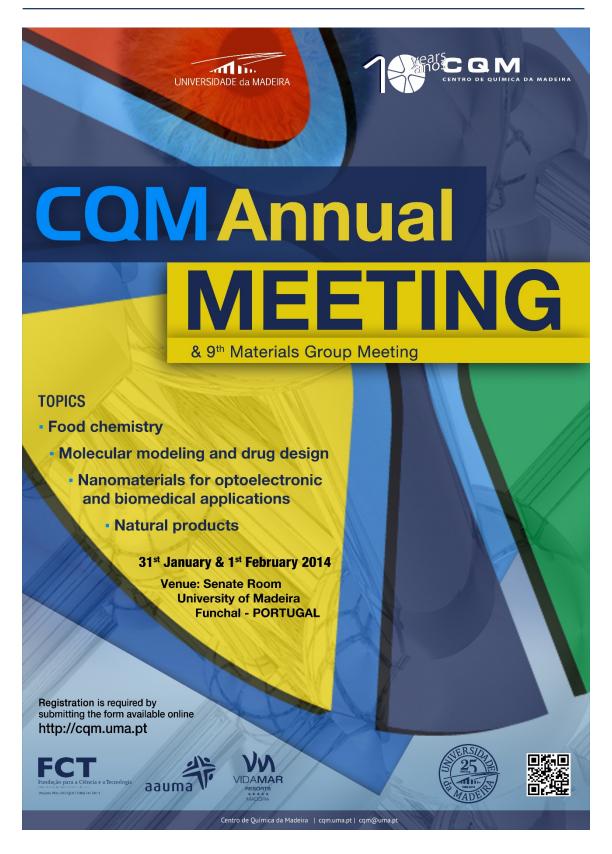




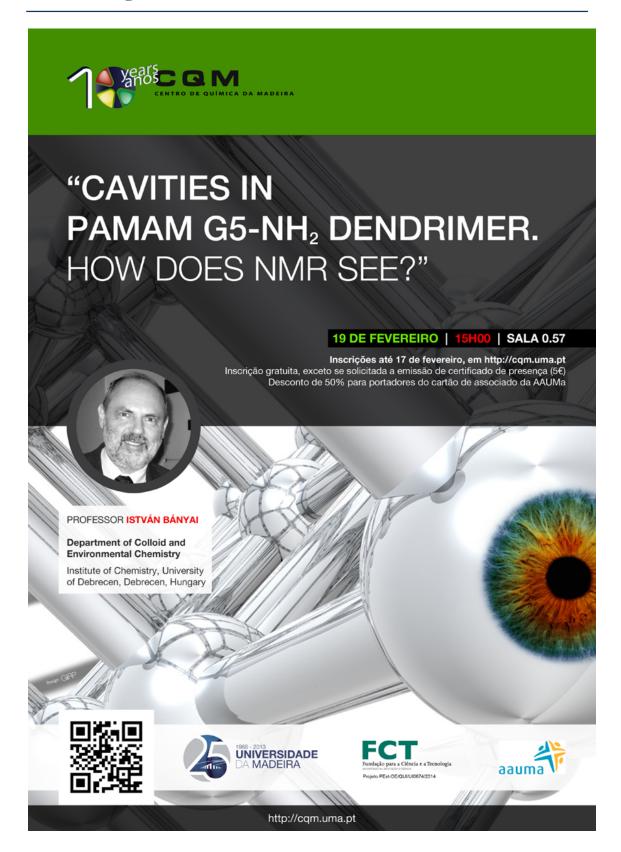
APPENDIX



















NOS LABORATÓRIOS DO CENTRO DE QUÍMICA DA MADEIRA

Para alunos universitários das áreas de BIOQUÍMICA, QUÍMICA e afins

ESTÁGIO 1

Entrega de genes em células animais

Supervisor: Helena Tomás Nº de vagas: 1

ESTÁGIO 2

Introdução às técnicas avançadas em Química Inorgânica

Supervisor: João Rodrigues

Nº de vagas: 2

ESTÁGIO 3

Liofilização de plantas, preparação de extractos vegetais e avaliação de actividade biológica

Supervisor: Paula Castilho

Nº de vagas: 2

ESTÁGIO 4

Desenvolvimento de uma nova estratégia analítica baseada na MEPS combinada com UHPLC-PDA para a quantificação de Sotolon em vinhos Madeira. Avaliação da correlação com a idade e com o tipo de vinho

Supervisor: José S. Câmara

Nº de vagas: 2

ESTÁGIO 5

Determinação de aminas biogénicas em vinhos fortificados com recurso a técnicas de microextração acopladas a cromatografia de alta eficiência. Estabelecimento da correlação do teor destes metabolitos com a idade do vinho

Supervisores: Jorge Pereira / José de Sousa Câmara № de vagas: 2



Candidaturas:

11 a 24 de junho de 2014, em http://cgm.uma.pt

Lista de candidatos selecionados:

25 de junho de 2014

Início dos estágios:

Entre 2 e 7 de julho de 2014 E-mail: cqm@uma.pt





















6 to 9 October 2014

University of Madeira, Funchal, Madeira

NANOSCHOOL COURSE

"Nanomedicines: Considerations for Design and Transfer into Clinical Use"

LESSON #01 MONDAY, 6TH | 15H00-17H00 | CONFERENCE ROOM 0.57

What is nanomedicine and why do we need it? Current Status of Nanomedicines in Clinical Use and Clinical Trial: Examples of Rationale for Design. Future Opportunities?

LESSON #02 TUESDAY, 7™ | 15H00-17H00 | CONFERENCE ROOM 0.57

Biological Barriers, Endocytosis and Intracellular Trafficking - Key Players that Determine Nanomedicine Performance - Safety and Efficacy. What are the Future Opportunities for Improved Nanomedicine Design?

LESSON #03 WEDNESDAY, 8TH | 14H30-16H30 | CONFERENCE ROOM 0.57

Designing Polymer Therapeutics as Anticancer Nanomedicines: Choice of the Polymer/Nanomaterial, the Drug, the Targeting Residue (± Imaging Agent), Considerations During Translation. How can we better Select Patients Most Likely to Respond To Nanomedicine Therapy? Opportunities for Design as Treatments for Other Diseases

LESSON #04 THURSDAY, 9TH | 15H00-17H00 | CONFERENCE ROOM 0.57

Translation of Nanomedicines from Lab to Clinical Practice: Nanotoxicology, Nanomedicines Regulation, and Ethical Considerations (Are Nanomaterials Safe or Dangerous?)

Registration required I from 2^{ND} July to 28^{th} September 2014 at http://cqm.uma.pt

OPEN CONFERENCE

WEDNESDAY, 8TH | 17H00-17H45 | CONFERENCE ROOM 'SALA DO SENADO'

"Nanomedicines: Fact of Fiction?"

Registration is not required for the conference











