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ABSTRACT BOOK





9th CQM Annual Meeting

Abstract Book

28-30 September 2022

Funchal, Madeira Island - PORTUGAL





Abstract Book of the 9th CQM Annual Meeting

Publisher

Centro de Química da Madeira

Address: Centro de Química da Madeira, University of Madeira, Campus da Penteada, 9020-105 Funchal (Portugal) Website: https://cqm.uma.pt Twitter: http://twitter.com/UMa_CQM Facebook: http://on.fb.me/gqSeD9 LinkedIn: http://bit.ly/LinkedIn_CQM Youtube: http://bit.ly/CQM_YouTube_Channel Instagram: https://www.instagram.com/centrodequimicadamadeira

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Rosa Perestrelo Énio Freitas

ISBN: 978-989-54090-6-8

The content of this publication can be used on the condition of full acknowledgement and citation of the source.







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About CQM

CQM is a National Research Unit and a *"refugee-welcoming organization*", supported by <u>FCT</u> (Unit 0674 - Ranking: Excellent), <u>ARDITI</u>, and <u>SRECT</u>.

Governance Structure

Executive Committee (2021-2022)

João Rodrigues	Scientific Coordinator
Pedro Pires	Materials Group Director
José S. Câmara	Natural Products Group Director

CQM Administrative and Technical staff

Emília Pimenta	Project Manager (UMa)
Énio Freitas	Board Assistant - Executive (UMa)
Paula Andrade	Administrative and Technical Staff (UMa)





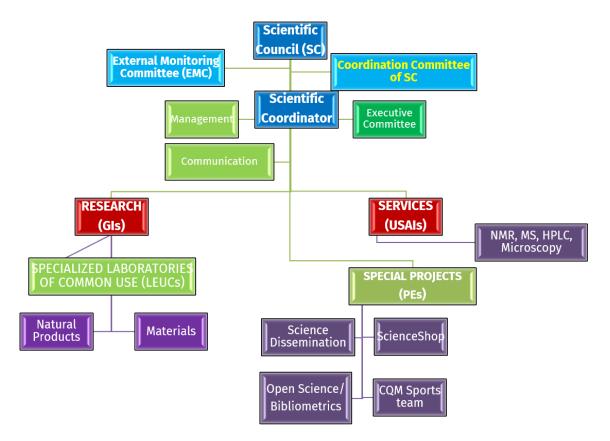
Permanent External Scientific Advisory Commission

José Martinho Simões	<i>Full Professor FCUL - Faculdade de Ciências, Universidade de Lisboa, Portugal</i>
Abhay Pandit	CÚRAM, Centre for Research in Medical Devices, National University of Irland
Makoto Fujita	<i>Full Professor, Department of Applied Chemistry, University of Tokyo, Japan</i>
John Beutler	<i>National Cancer Institute - Center for Cancer Research, USA</i>
Jean-Pierre Sauvage (2016 Nobel Prize in Chemistry)	<i>Institut de Science et d'Ingénierie Supramoléculaires, University of Strasbourg (France).</i>





Organizational Structure







Vision and Mission

Our Vision

Making the CQM a renowned research institution in the field of Natural Products and Materials.

Our Mission

CQM - Centro de Química da Madeira/Madeira Chemistry Research Centre - constitutes a central element in the promotion and enlivening of R&D activities in the field of Chemistry and Biochemistry in the Autonomous Region of Madeira, Madeira Island, Portugal. CQM is firmly committed in the development of advanced training, partnerships with national and international institutions, the offer of services to the community and in the popularization of science.

Our Philosophy

To be a relevant part of a scientific community that performs world-class research aimed at improving the scientific knowledge and the well-being of Society.

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, each one representing various areas of chemistry and biochemistry, working together to improve scientific knowledge and contribute to the well-being of Society.







CQM Commitments and Principles

CQM follows the Code of Conduct from the University of Madeira, the rules of the Fundação para a Ciência e a Tecnologia (FCT-IP), the European Charter for Researchers, the Code of Conduct for the Recruitment of Researchers (Commission Recommendation, Brussels, 11.3.2005, 2005/251/EC) since 2008, and the recommendations from the San Francisco Declaration on Research Assessment (DORA) being committed to the principle of equity in employment and selection based on merit, non-discrimination in respect of gender, age, nationality, religion, racial group, or any other possible discriminatory issue.

CQM is strongly committed to all the European regulations related to the ethical, legal and social aspects (ELSA) and governance of nanotechnology, namely with the COMMISSION RECOMMENDATION of 07/02/2008. CQM also voluntarily 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, and the existence of a cell culture facility at CQM allows for the biological evaluation of the developed materials in Madeira (*e.g.,* cytocompatibility studies, gene delivery studies). In particular, adult human stem cells are being used in the studies with the authorization of the Local Ethical Committee and also respecting the national and European rules.





CQM - The Crossroad



Throughout more than 18 years of work as an FCT research unit, CQM has assumed, as its strategic objective, to assert itself nationally and internationally in two major scientific areas: natural products and materials. CQM has developed a high organizational exigency policy to achieve these objectives, investing all funds obtained through competitive calls in infrastructure, equipment, and human resources. The result of this strategy was reflected in the results of the latest external and

international evaluation of the FCT research units completed in 2021. For the first time, a research center entirely based in the Autonomous Region of Madeira gets the **EXCELLENT** classification. However, this result is not the result of episodic work. As in war, the final victory results from many battles, advances, and retreats, and of course, more victories than defeats.

The trajectory of CQM as a research unit is the result of consistent and sustained work that, despite the pandemic, was unequivocally reflected in the work done in 2021 and already in 2022. Therefore, in 2021, the CQM published 71 articles in journals, with impact factor (Figure 1) being 76% of the articles published in journals of the first Quartile and 22.5% of the first Decile. In addition, 5 other publications were published as books/book chapters and articles in journals without impact factor. Regarding the publications for this year, the projection also points to values very close to those of previous years.

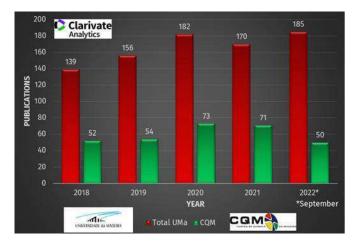


Figure 1 - CQM publications from 2018-2022*(Only articles in journals with impact factor).

Nevertheless, the work of CQM is not only evaluated by the metrics of publications (number of publications, impact, citations). Thus, 5 Ph.D. and 7 MSc students completed their training at CQM in 2021. Also, in 2021, it is important to highlight the employment contract of Dr. Ruilong Sheng, approved under the *FCT's Incentive Scheme for Individual Scientific Employment - 4th Edition*. Furthermore, we are very proud that for the first time, 5 of our researchers, 2 of them in their early careers, Dr. Rosa Perestrelo and Dr. Jaison Jeevanandam, joined the "World's Top 2% Scientists list", a list of the most





cited researchers worldwide in different areas of knowledge, organized by Stanford University and the publisher Elsevier BV* (Figure 2).



Figure 2. CQM reserachers on the World's Top 2% Scientists list (2021).

If the results presented are due to the working capacity and resilience of our human resources, the human capital of the CQM is an asset that, as defined in our strategic plan 2018-2022, must be preserved and strengthened.

As stated elsewhere, we do not foresee being able to maintain the level of evaluation achieved and contribute to the national and regional smart specialization strategy, nor be financially sustainable without:

(a) a stable team of 20-25 Ph.D. holders, corresponding to 16-18 full-time equivalent (FTE) Ph.D. holders, with employment contracts and research grants;
b) a permanent technical/administrative and dissemination/promotion team;

c) investing in the renovation of spaces and equipment;

d) continuing to have the capacity to attract highly qualified human resources in the national and international market that complement the existing critical mass and bring more scientific and financial value to the CQM and the Region.

Unfortunately, "the year of all dangers" has not passed, and CQM is now, in terms of human resources, less prepared than in the past to face the next external and international evaluation of R&D units promoted by FCT. Although there is funding available at CQM that can minimize the loss of highly qualified human resources, our predictions indicate that in September 2023, the CQM will have 11 fewer Ph.D. holders than in December 2021. From the current 14.5 FTE, we will go to 7.9 FTE in 2023, a number below the minimum accepted by FCT for a research unit to compete in the following external and international evaluation of R&D units.

In fact, and although many of these human resources who have finished (or will soon finish) their connection with CQM wish to continue working with us if they have that opportunity, there are several difficulties encountered, namely:





a) the Decree Law No. 123/2019 that, in its article 2, number 2, paragraph a), prevents the hiring, through post-doctoral fellowships, of Ph.D. holders who have carried out their Ph.D. at the same host institution,

b) the Regulation for Evaluation and Pluriannual Financing of Research Units approved this year (Regulation 404/2022), namely its article 6, number 4, which obliges "each R&D unit to incorporate integrated doctoral researchers with a minimum of ten FTE",

c) the limitations that the CQM's host institution, the University of Madeira, has placed on the launch of calls for tender for employment contracts,

d) and also the fact that, in all these years, we have never been covered by any application submitted by UMa involving our researchers under the Institutional Scientific Employment Incentive Tender - even when situations resulting from the non-application to researchers of the CQM of the transitional rule of DL no. 57/2016, as amended by Law no. 57/2017, are still to be solved.

These constraints will seriously limit or prevent the CQM from applying for the following external and international evaluation of research units. As a result, not only is all the work and investment done at the CQM at risk of being wasted, but the absence of an FCT Center in the area of Chemistry and Biochemistry in Madeira and at UMa jeopardizes the survival of the 4 existent courses in the area. Additionally, it will be more difficult to apply for funding for research projects and to participate in national and international research networks and scientific infrastructures. The University of Madeira will also cease receiving the overheads due to the different research projects in which CQM and its researchers participate.

The possible consequences of this situation, for which, as Coordinator of the CQM, I warned very early on, are pretty straightforward. Above all, what worries me is not only to see the investment of almost two decades being unnecessarily wasted but also to see that the effort and dedication of the researchers at the CQM will not be rewarded. In particular, I am concerned about the future of the younger researchers who took the greatest risks and are now in danger of seeing their life goals frustrated and their legitimate career aspirations at the Center canceled. That said, as has been our motto, we will continue to battle in the certainty that what is in our hands will be done. As long as we exist, we will be here to fulfill our mission, to serve the University of Madeira, the Region, and the Country!

University of Madeira, Funchal, 28th of September 2022

(João Rodrigues, Scientific Coordinator of CQM)







[O] Oral Communitation [FP] Flash Presentation

Wednesday, 28th September 2022

09:15 09:45 Participants Registration

Opening Session Sílvio Fernandes Rector of the University of Madeira Jorge Carvalho Regional Secretary of Education, Science and Technology Francisco Fernandes President of the General Council of the University of Madeira 09:45 10:30 Madalena Alves President of the Portuguese Foundation for Science and Technology - FCT Rui Caldeira President of the Administration Council of ARDITI José Manuel Baptista President of the Faculty of Exact Sciences and Engineering João Rodrigues Scientific Coordinator of CQM

10:30 11:00 Coffee-break

Chair: Jorge Pereira [O-01] Hydrogels as biomimetic materials for cancer immunotherapies 11.00 11:40 Fabião Santos [FP-01] Effects of oxidation on the fluorescence and biological properties of 11:40 11:45 Nanomaterials for biomedical applications - a Summer Internship Oriana Lozano, Lydia dos Orfaos, Rita Castro & João Rodrigues [FP-02] Spectral simulation of picogreen 11:50 11.45 Francisca Viveiros & Pedro Pires [FP-03] 11:50 11:55 (Speaker did not attended the meeting) [FP-04] Cardoon extracts: Determination of antioxidant activity 11:55 12:00 Carolina Costa, Joana Pinto & Paula C. Castilho [O-02] Urinary metabolomic fingerprints as a powerful tool for the next generation of 12:00 12:15 prostate cancer diagnosis Cristina V. Berenguer, Ferdinando Pereira, Jorge A.M. Pereira & José S. Câmara [O-03] Fucoidan-based delivery system for cisplatin in glioblastoma cells 12:15 12:30 Ana Duarte, Filipe Olim & Helena Tomás 12:30 12:35 9th CQM Annual Meeting Photo





12:35 14:00 Lunch

Chair: Rita Castro		
14:00	14:30	[O-04] Cellulose extraction and nanocellulose preparation from invasive <i>Arundo donax</i> L. plant leaves Jaison Jeevanandam & João Rodrigues
14:30	14:55	[O-05] Potential targets of caffeoylquinic acids in the human tricarboxylic acid cycle <u>João Serina</u> , Paula C. Castilho & Visvaldas Kairys
14:55	15:20	[O-06] The effect of the reaction time on the synthesis of fluorescent carbon dots <u>Ivo Martins</u> & João Rodrigues
15:20	15:35	[O-07] Bioprospection of bioactive compounds from coffee waste biomass as a useful strategy for its valorization <u>Carolina Andrade</u> , Rosa Perestrelo & José S. Câmara
15:35	16:00	[O-08] Fucoidan/dendrimer nanoparticles and their angiogenic properties <u>Filipe Olim</u> , Ana Rute Neves, Irene Rodriguez-Clemente, Valentín Ceña & Helena Tomás
16:00	16:25	[O-09] Polyphenolic profile and antioxidant potential of different morphological parts of <i>Corema album</i> <u>Joana Pinto</u> & Paula C. Castilho

Thursday, 29 th September 2022		
Chair: 3	Jaison J	leevanandam
09:30	10:10	[O-10] Green Biomaterials (III): Natural steroid-based nanobiomaterials for gene/drug delivery Ruilong Sheng
10:10	10:35	[O-11] Sequential extraction of pectin and hesperidin from orange peel wastes: A green chemistry approach <u>Onofre Figueira</u> , Verónica Pereira & Paula C. Castilho
10:35	11:00	[O-12] Synthesis of linear dendritic block copolymers based on bis-MPA with bone targeting capability for osteosarcoma treatment <u>Fátima Mendes</u> , Natalia Sanz del Olmo, Jorge San Jacinto Garcia, Michael Malkoch & Helena Tomás
11:00	11:30	Coffee-break
11:30	11:55	[O-13] Discards from legumes as bacteria cryoprotectants Gonçalo N. Martins, <u>Angela D. Carboni</u> , Ayelén A. Hugo, Andrea Gómez-Zavaglia & Paula C. Castilho
11:55	12:10	[O-14] Synthesis and characterization of fluorescent carbon dots from <i>Ricinus</i> <i>communis</i> L. <u>Filipa Pita</u>, Ivo Martins & João Rodrigues
12:10	14:00	Lunch
Chair: Ruilong Sheng		
14:00	14:25	[O-15] <i>(Speaker did not attended the meeting)</i>





14:25	14:40	[O-16] Spheroid development for in vitro chondrogenesis – Preliminary studies <u>Filipa Jardim</u> , Mara Gonçalves & Helena Tomás
14:40	15:05	[O-17] Oxidation of fluorinated PAMAM dendrimer – A combination of fluorescence and NMR traceability Lydia dos Orfaos, Helena Tomás & João Rodrigues
15:05	15:20	[O-18] NOVAearth: A solution to wash the hands which will reduce plastic and use agri-food waste Henrique Sousa, <u>Duarte Fernandes</u> & João Firmino
15:20	15:50	Closing Session

Friday, 30th September 2022

14:30 18:00 MACARONIGHT - Visit to CQM labs





Flash Presentations





[FP-01]

Effects of oxidation on the fluorescence and biological properties of nanomaterials for biomedical applications – a summer internship

Oriana Lozano. Lydia dos Orfaos, Rita Castro & João Rodrigues*

CQM-Centro de Química da Madeira, MMRG, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal.*joaor@uma.pt.

During this internship, I have been involved in the PhD work of the student Lydia dos Orfãos. In this work, synthesis and oxidation reactions, using ammonium persulfate, were carried out in the functionalized PAMAM dendrimers with 4-hydroxybenzoic acid and 2,3,5,6-tetrafluoro-hydroxybenzoic acid. The products obtained were dialyzed, lyophilized, and, subsequently, characterized using the following techniques: nuclear magnetic resonance (NMR), UV/Vis spectroscopy, and fluorescence spectroscopy.

Furthermore, guided by Dr. Rita Castro, I performed *in vitro* cytotoxicity studies in human embryonic kidney (HEK) cells to evaluate the cytotoxicity effects of polyethyleneimine and halloysite/chitosan complexes conjugated with DNA. HEK cells were exposed to different concentrations of conjugated complexes for 48 hours. In order to evaluate the cytotoxicity effects, we resorted to: fluorescence microscopy, resazurin test, and quantification of proteins using the bicinchoninic acid method.

In conclusion, this internship allowed me to live the daily life of a research center, learn new techniques of analysis and structural characterization only available at CQM, broaden my scientific knowledge in areas internationally recognized, and, not least, establish contacts that could be useful to me in the future.

Acknowledgments: The authors acknowledge the support of FCT-Fundação para a Ciência e a Tecnologia through the CQM Base Fund UIDB/00674/2020, Programmatic Fund UIDP/00674/2020, and Secretaria Regional de Educação, Ciência e Tecnologia, through ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação. OL truly appreciated CQM-Centro de Química da Madeira for the conditions offered and the Direção Regional de Juventude, through the Summer Internship Program for university students, for funding this internship.





[FP-02]

Spectral simulation of picogreen

Francisca Viveiros & Pedro Pires*

CQM-Centro de Química da Madeira, Campus Universitário da Penteada, 9020-105, Funchal, Portugal. *pedro.pires@staff.uma.pt.

PicoGreen is one of the most relevant molecules in biomedical research, and it has been successfully applied in the quantification of DNA in solution and in other techniques due to the increase in fluorescent emission after interaction with DNA. In order to better understand the mechanism for the fluorescence enhancement, we performed a molecular modelling study of the PicoGreen-DNA interaction. Initially, we built a PicoGreen model, then the DNA strand and finally we proceeded with its intercalation. This intercalation was done with the Amber 99 molecular mechanics method. We obtained the absorption and emission spectra for PicoGreen + Water and for PicoGreen + Water + DNA and their respective energy diagrams. For the calculation of the spectra, we used the semi-empirical quantum mechanics method RM1, in the ground state and in the excited state, optimizing the geometries with a gradient of approximately 1 kcal/(A.mol). The wavelengths of the maximum absorption and emission calculated for the PicoGreen + Water + DNA, we similar to the experimental values obtained in the literature. Finally, we analyzed the frontier molecular orbitals and verified the existence of a strong interaction between the PicoGreen orbitals and the purine and pyrimidine rings of DNA. This interaction might be responsible for the fluorescence increase of the intercalated PicoGreen, when compared to the free molecule.

For future studies, it would be interesting to carry out more intercalations and also carry out these experiments in more refined quantum mechanics methods, such as DFT or the Ab Initio method.

Acknowledgments: The authors acknowledge the support of FCT - Fundação para a Ciência e a Tecnologia through the CQM Base Fund - UIDB/00674/2020, Programmatic Fund - UIDP/00674/2020, Ingress® and Secretaria Regional de Educação, Ciência e Tecnologia, through ARDITI - Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação.



Cardoon extracts: Determination of antioxidant activity

Carolina Costa, Joana Pinto & Paula C. Castilho*

<u>OM ANNUAL</u>

EETING

CQM-Centro de Química da Madeira, Campus Universitário da Penteada, 9020-105, Funchal, Portugal. *pcastilho@staff.uma.pt.

Phenolic compounds are secondary metabolites produced by plants and other organisms that affect animal biological systems. They have a huge medical and therapeutic importance, mainly due to their antioxidant capacity. Therefore, they react with free radicals (reactive oxygen and nitrogen species), naturally produced during cellular respiration or by exogenous action, preventing diseases associated with oxidative stress such as diabetes (1). In this study, four species of cardoon were analysed for their total phenolic and flavonoid contents and antioxidant activity by DPPH method. Cardoon species were collected from the wild. Phenolic compounds were extracted by ultrasonic bath using methanol as solvent, which was concentrated to dryness under reduced pressure. The dried extracts were diluted for subsequent execution of the assays of TPC (Total Phenolic Content), TFC (Total Flavonoid Content) and DPPH (2,2-diphenyl-1-picrylhydrazyl). Hence, various calibration curves with different compounds (gallic acid, quercetin and trolox) were drawn and the absorbance was measured. The results were obtained by interpolation and expressed in appropriate units. The antioxidant assays showed significant differences between the analysed species.

Additionally, cardoon extracts were submitted to phytochemical profile determination by HPLC-ESI-MSⁿ. In this context, this work can contribute for the knowledge and characterization of cardoon species.

References:

[1] Pinto, J.C. 2016. Estudo da composição e das propriedades bioactivas de plantas produtoras de bagas. [Master's Dissertation, University of Madeira].

Acknowledgments: This work was supported by FCT-Fundação para a Ciência e a Tecnologia through the CQM Base Fund - UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020, and by ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação, through the project M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM+(Madeira 14-20 Program).





Oral Communications





[0-01]

Hydrogels as biomimetic materials for cancer immunotherapies

Fabião Santos

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Recent achievements in the field of immunotherapy, such as the development of engineered T cells used in adoptive cell therapy, are introducing more efficient strategies to combat cancer. Nevertheless, these T cells are challenging to manufacture, manipulate, and control. Specifically, there are limitations in producing the large amounts of specific T cells needed for these therapies in a short period of time and in an economically viable manner.

During my PhD studies, we have studied different 3D systems with the objective of achieving higher proliferation rates and tune the resulting phenotypes, by resembling the natural environment of the secondary lymphoid organs.

Acknowledgments: Prof. Jaume Veciana (ICMAB), Dr. Imma Ratera (ICMAB), and Dr. Judith Guasch (ICMAB).





[O-02]

Urinary metabolomic fingerprints as a powerful tool for the next generation of prostate cancer diagnosis

Cristina V. Berenguer¹, Ferdinando Pereira², Jorge A. M. Pereira¹ & José S. Câmara^{1,3,*}

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Despite the spectacular advances in molecular medicine, including genomics, proteomics, transcriptomics, lipidomics, and personalized medicine, prostate cancer (PCa) remains the most frequent malignant tumour and a leading cause of oncological death in men. Apart from classical biomarkers, the study of endogenous volatile organic metabolites (VOMs) biosynthesized by different metabolic pathways and found in several biofluids is emerging as an innovative, efficient, and non-invasive source of data to establish the volatilomic biosignature of PCa patients. In this context, the primary objective of this work was to establish the urinary volatilomic profile of PCa using headspace solid-phase microextraction combined with gas chromatography-mass spectrometry (HS-SPME/GC-MS). This non-invasive approach to set putative PCa biomarkers was applied to PCa patients (n = 29), men subjected to radical prostatectomy (RP, n = 34), and cancer-free individuals (control group, n = 49). A total of 60 VOMs belonging to different chemical families were identified in the groups under study. The data matrix obtained was submitted to multivariant analysis, through partial least-squares discriminant analysis (PLS-DA). The results obtained did not show complete discrimination between the groups under study, since more than 50% of the variability obtained could not be explained by the models. The heatmap according to Pearson's correlation showed that 2-(1cyclopentyl)furan, 2-pentanone and 2-bromophenol were more associated with the control group, while carvone, α -corocalene, 2-acetylfuran, and cyclohexanone showed high correlations with the PCa group. In contrast, 2-ethyl-5-methylfuran, methanethiol, o-methoxyphenol, pcymenene, and 3,4-dehydro- β -ionene, were more associated with the RP group. An exhaustive study of the demographic and clinical characteristics of the patients recruited and a larger cohort of samples are crucial to elucidate the changes that occur in the volatilomic profiles.

Acknowledgements: This work was supported by FCT-Fundação para a Ciência e a Tecnologia, through the CQM Base Fund - UIDB/00674/2020 and Programmatic Fund - UIDP/00674/2020, and by ARDITI -Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação, through the project M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM+ (Madeira 14-20 Program) and the Post-Doctoral fellowship given to JAMP (Project M1420-09-5369-FSE-000001). CVB acknowledges Núcleo Regional da Madeira da Liga Portuguesa Contra o Cancro (LPCC-NRM) and Bolsa Rubina Barros for the support of this project. The authors also acknowledge the financial support from FCT and Madeira 14-2020 program to the Portuguese MS Network through PROEQUIPRAM program, M14-20 M1420-01-0145-FEDER-000008.





[0-03]

Fucoidan-based delivery system for cisplatin in glioblastoma cells

Ana Duarte, Filipe Olim & Helena Tomás*

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As one of the most prominent diseases nowadays, cancer has been the focus of much of the research in the scientific community in the last few decades. Nanomaterials may present a lot of advantages to cancer therapy, particularly as drug delivery systems. Due to their reduced size, they display high bioavailability and facilitated cell uptake mechanisms, and they can encapsulate or be conjugated to drugs [1]. Moreover, nanomaterials are potentially able to deliver drugs to specific targets in a controlled release mode, which reduces the drug's adverse side-effects. Several materials, such as polymers (including dendrimers), inorganic nanoparticles, liposomes, for example, have been utilized for the design of these delivery systems [2].

In this work, a fucoidan-based delivery system for cisplatin, an anticancer metallodrug, was designed. The nanoparticles were synthesized through a self-assembled process with two types of fucoidan (extracted from Fucus vesiculosus and Undaria pinnatifida), a dendrimer based on the bis-MPA monomer, and cisplatin. The nanoparticles were characterized by DLS/ELS for measurement of their hydrodynamic diameter and zeta potential. Their cisplatin loading efficiency was determined, as well as their cytotoxicity using the U-87 MG cell line (often used as a model of glioblastoma). Additionally, the hemotoxicity of the nanoparticles was evaluated and the cisplatin release profile in distilled water was assessed. It was observed that the nanoparticles present drug loading efficiencies that could be related with their sulfate content. Their hydrodynamic diameter and zeta potential reflected the nanoparticle composition and the presence of cisplatin. Their cytotoxicity level in the U-87 MG cells was not very high and most assays did not cause the death of 50% of the cells for the range of studied concentrations. Moreover, their hemotoxicity was shown to be low, and preliminary cisplatin release profile studies showed evidence of sustained release behaviour. In summary, the delivery system designed in this study displayed promising results, although many more variables need to be assessed for this system to be considered viable.

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Acknowledgements: The authors acknowledge the support of FCT-Fundação para a Ciência e Tecnologia through Portuguese government funds - projects UIDB/00674/2020 (base funding) and UIDP/00674/2020 (programmatic funding). Additionally, Marinova Pty Ltd (Tasmania, Australia) contribution with the fucoidan samples is also acknowledged. FO thanks ARDITI for the Ph.D. fellowship M1420-09-5369-FSE-000002.





[O-04]

Cellulose extraction and nanocellulose preparation from invasive *Arundo donax* L. plant leaves

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Invasive plants are non-native species that can rapidly spread in a specific geographic location, These plants utilize most of the nutrients from the soil and reduce native plant growth, which can affect the ecosystem balance. Hence, it is essential to control invasive plant growth to avoid critical ecosystem damage. Generally, chemical, mechanical, and biological methods are used to control the growth of invasive plants. However, the disadvantages of these methods, such as environmental toxicity, nutrient cycle disturbance, and genetic integrity loss, limit their large-scale applications [1,2]. Therefore, utilization of these invasive plants to extract valueadded products will be beneficial to reuse and reduce them, thereby protecting the native plants and ecosystems. Arundo donax L. (common name: giant cane or giant Reed) that are native of Asia and typically known in Portugal as Cana Vieira, is an invasive plant on Madeira Island. Traditionally, these plants are used as crop support, construction of heat-insulating roofs, and to make wind and musical instruments. The leaves were identified to possess 31-49% of cellulose, 22-35% of hemicellulose, and 9-22% of lignin [3-4]. Thus, we aim to extract pure cellulose from the leaf powder of A. donax and prepare nanocellulose using organosolv fractionation, bleaching, and centrifugal fractionation approach. The results showed that the yield of cellulose from the leaf powder is 40%. The systematic characterization showed that the crystallinity of the cellulose in each stage of the extraction process and the nanocellulose were 91.2 nm of average particle size with 0.428 of polydispersity and -35.5 mV of zeta potential. Further, the morphology analysis results indicated the presence of a fibrous matrix with a cube and quasi-spherical shaped nanocellulose of \geq 100 nm size.

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[0-05]

Potential targets of caffeoylquinic acids in the human tricarboxylic acid cycle

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The tricarboxylic acid cycle (TCA), often referred to as Krebs cycle, is an essential pathway in energy metabolism and is the nexus to other energy specific pathways and to both amino acid and fatty acid metabolisms. Caffeoylquinic acids (CQAs) are plant secondary metabolites, which have been shown to affect several enzymes and pathways associated with carbohydrates and energy production/consumption in mammals. These compounds have been shown to restore the activity and or expression of enzymes in some of these pathways to near homeostasis levels and, despite having some known targets and verified effects, the generalized mechanism of action for CQAs remain elusive. To find potential targets, 32 structures of 16 human enzymes in the TCA were used as receptors in molecular docking simulations with CQAs being studied as ligands. Statistically significant differences were found in the binding affinity results for all enzymes, with pyruvate carboxylase, succinate dehydrogenase and phosphoenolpyruvate carboxykinase having the top three best performing results. As observed in our previous work, CQAs appear to bind more favorably to the binding sites of phosphorylated nucleoside cofactors such as ATP/ADP, NAD(P)⁺, GTP or FAD.

Acknowledgments: This work was supported by Fundação para a Ciência e a Tecnologia (Base Fund -UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020), and by ARDITI - Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação, through the project M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM⁺ (Madeira 14-20 Program).

João Serina would like to acknowledge FCT for the PhD grant 2020.05328.bd and the Vilnius University for the use of the High-Performance Computer Cluster at the Bioinformatics Department of the Life Sciences Center.





[0-06]

The effect of the reaction time on the synthesis of fluorescent carbon dots

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During the last decade, carbon dots (CDs) have gained particular interest in the research community due to their properties and potential applications [1]. CDs are photoluminescent (PL) nanosized particles between 1-20 nm, mainly composed of carbon and from heteroatoms like O. N, or S, located on the internal structure or at the surface and highly responsible for their PL properties [2]. These CDs are mainly synthesized by combining the hydrothermal method, carbon-rich starting precursors, and selecting the best reaction parameters like temperature and time. In fact, a substantial part of the research work has been devoted to the synthesis of CDs with superior PL properties employing proof-of-concept methods and countless starting materials [3], but little attention was given to the influence of reaction parameters such as time, temperature, concentration, and type of solvent on the CDs yield and final PL properties. Therefore, we propose the use of a systematic approach to try to reach control of the size, surface composition, yield, and PL properties, as well as reproducible CDs for future applications. In this work, the influence of the reaction time on the synthesis of CDs was studied using the hydrothermal method, ascorbic acid as the precursor, static temperature, and varying the synthesis time. After synthesis, the reaction products were purified by centrifugation and dialysis and lyophilized to estimate the synthesis yield and further characterization. These reaction products were characterized using UV-Vis, fluorescence, and NMR spectroscopies, as well as TEM and DLS, and all these results will be presented and discussed.

Representation of the hydrothermal synthesis.



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Acknowledgments: The authors acknowledge the support of FCT-Fundação para a Ciencia e a Tecnologia (Base Fund UIDB/00674/2020 and Programmatic Fund UIDP/00674/2020, Portuguese Government Funds), and the Ph.D. grant 2021.05990.BD (Ivo Martins). The support of Secretaria Regional de Educação, Ciência e Tecnologia, through ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação is truly appreciated.





[0-07]

Bioprospection of bioactive compounds from coffee waste biomass as a useful strategy for its valorization

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Coffee is one of the most popular beverages in the world and its consumption generates copious amounts of waste. Although generally treated as waste, spent coffee grounds are a rich source of several bioactive compounds, with applications in diverse industrial fields. The present work aimed the analysis of spent coffee grounds from different geographical origins for the identification of bioactive compounds with industrial interest. For this purpose, the volatile fingerprint was established by headspace solid-phase microextraction coupled with gas chromatography mass spectrometry (HS-SPME/GC-MS). Additionally, the bioactive and antioxidant potential was assessed through a µ-QuEChERS methodology coupled to spectrophotometric techniques (total phenolic content (TPC), and DPPH and ABTS scavenging assays). Finally, the identification of the bioactive compounds responsible for the antioxidant activity attributed to the spent coffee grounds was attempted, using miniaturized solid-phase extraction (µ-SPEed) coupled to ultrahigh performance liquid chromatography with photodiode array detection (UHPLC-PDA). The volatile fingerprint analysis enabled the identification of a total of 111 volatile organic compounds (VOCs) in the spent coffee grounds belonging to different chemical families. Furanic compounds, nitrogen compounds, esters, carbonyl compounds, volatile phenols, and terpenoids comprised most of the volatile fingerprint. Some of the major VOCs identified have been reported in literature to have great potential as raw material for applications in food and non-food products. The highest value for the TPC was obtained for the sample from Brazil (53.68 ± 3.120 mg GAE/100 g DW), while Colombia presented the lowest value (41.56 ± mg GAE/100 g DW). As for the DPPH assay, the highest scavenging activity was presented by Brazil (78.11 ± 7.333 mg TE/100 g DW) and the lowest for Guatemala (50.64 ± 5.257 mg TE/100 g DW). Finally, the UHPLC-PDA analysis permitted the identification and quantification of seven bioactive compounds in the spent coffee grounds. The results obtained in this work show that spent coffee grounds are a rich source of several bioactive compounds, supporting its bioprospection based on circular economy concept closing the loop of coffee value chain, toward the valorisation of coffee by-products.

Acknowledgments: This work was supported by FCT-Fundação para a Ciência e a Tecnologia through the CQM Base Fund–UIDB/00674/2020, and Programmatic Fund–UIDP/00674/2020, and by Madeira 14-2020 Program, to the Portuguese Mass Spectrometry Network (PROEQUIPRAM, M14-20 M1420-01-0145-FEDER-000008), by ARDITI–Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação, through the projects M1420-01-0145-FEDER-000005–Centro de Química da Madeira–CQM⁺ (Madeira 14-20 program).





[O-08]

Fucoidan/dendrimer nanoparticles and their angiogenic properties

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The formation of new vasculature constitutes an important process, for example in wound healing and tissue regeneration. However, in the scope of cancer, it can contribute to significant changes in the tumour features, leading to its progression and capability to metastasize in distant places. Among different types of cancer, glioblastoma, a severe type of brain cancer, is characterized by having a high vascular density. There are some formulations in the market such as Avastin (Bevacizumab) that target angiogenesis, but patients can experience some side effects and its efficacy is still questionable. For these reasons, the development of new strategies targeting angiogenesis may enormously benefit patient's treatment [1]. Fucoidans are a class of sulfated polysaccharides mainly extracted from brown algae. They have been shown to exert various biological activities, including pro- or anti-angiogenic effects depending on their structural features [2].

The main aim of this work was to prepare and characterize fucoidan/dendrimer nanoformulations and further study their angiogenic properties. First, through the *in vitro* tube formation assay, it was possible to assess the *in vitro* pro- or anti-angiogenic properties of fucoidans from two different algae species (*Fucus vesiculosus* and *Undaria pinnatifida*), as well as of their respective hydrolysed counterparts. The non-hydrolysed polysaccharides presented the best anti-angiogenic response so therefore were selected for integration in nanoparticles based on fucoidan and bis-MPA-based degradable dendrimers. The nanoparticles were prepared at different ratios and characterized. After determining the best fucoidan:dendrimer ratio for the nanoformulations, their pro-angiogenic activity was evaluated both *in vitro* and *in vivo*. Results showed that the nanoformulations can also exert anti-angiogenic activity.

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[O-09]

Polyphenolic profile and antioxidant potential of different morphological parts of *Corema album*

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Corema album (L.) D. Don (*Ericaceae*) is an endemic shrub that can be found in Southern European Atlantic coastal dunes. The fruit is a spherical berry white or pinkish white when ripe and contain reddish seeds (Portuguese white crowberries or "*camarinhas*" in Portuguese). The fruit have been traditionally consumed in these coastal areas, fresh or after processing form (lemonade, jam, liqueur)¹.

Even though this plant has attracted the interest of the scientific community in recent years, there are not much published research on it. In this sense, the present study assessed the phytochemical profile and antioxidant potential of various morphological parts of *C. album*, including leaves, berries, seeds, and flowers.

HPLC-DAD-ESI/MSⁿ was used to determine the phenolic profile of the different morphological components of the *C. album* in both the negative and positive modes. Thirty-seven compounds were tentatively identified.

In *C. album* leaves and flowers, epicatechin, proanthocyanidins and *O*-glycosilated flavonols (derivatives of quercetin, kaempferol and laricitrin) are predominant. Phenolic acids, such as caffeoylquinic acids, and *O*-glycosilated flavonols are an important constituent of berries and seeds. Only a little amount of anthocyanins was detected in the fruit pulp extract using positive mode analysis.

The total phenolic and flavonoids contents showed that leaves have higher values, compared to berries pulp, the extract from seeds is much richer in phenolic and flavonoid contents.

Overall, all performed experiments revealed that leaves extract had greater antioxidant potential.

This study offers a contribution for the phytochemical characterization and a consequent valorization of *Corema album* species.

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Joana Pinto is the recipient of FCT Ph.D grant 2020.08352.BD. The authors are grateful to IDEAS4life project for the supply of C. album extracts.





[0-10]

Green biomaterials (III): Natural steroid-based nanobiomaterials for gene/drug delivery

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Using natural steroid compounds to construct functional polymer nanomaterials for the biomedical application toward the treatment of cancer can bring many advantages [1]. In this work, we developed two steroid-based polymer gene/drug delivery systems: 1). A series of steroid-based cationic random copolymers (PMA6Chol-r-PDMAEMA and PMA6Dios-r-PDMAEMA) were synthesized using RAFT polymerization, which could self-assemble with pDNA into size-tunable nanoparticles and have low apparent cytotoxicity within pDNA transfection concentration range, PMA6Dios-r-PDMAEMA showed higher pDNA transfection capabilities PMA6Chol-*r*-PDMAEMA at high hydrophobic ratio. Moreover, PMA6Chol-rthan PDMAEMA/pDNA and PMA6Dios-r-PDMAEMA/pDNA demonstrated different intracellular localization properties [2]; 2). A cholesterol-based glycopolymer PMAgala-b-P(MAA-co-MAChol) was facilely prepared by RAFT polymerization and following TFA deprotection, the Doxloaded PMAgala-b-P(MAA-co-MAChol) nanomicelles have good biocompatibility and pHresponsive Doxorubicin releasing property. Dox-loaded PMAgala-b-P(MAA-co-MAChol) micelles enter the cell mainly through the clathrin/ caveolae-mediated endocytic pathway and can cause up-regulation of autophagy. Regulating the autophagy process is an efficient way to enhance drug delivery efficiency of Dox-loaded PMAgala-b-P(MAA-co-MAChol) glycopolymers [3].

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Acknowledgments: This work was supported by FCT-Fundação para a Ciência e a Tecnologia through the CQM Base Fund - UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020, and by ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação, through the project M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM⁺ (Madeira 14-20 Program)." We also thank FCT individual employment grant 2021.00453.CEECIND and ARDITI fellowship grant ARDITI-CQM-2017-003-ISG.





[0-11]

Sequential extraction of pectin and hesperidin from orange peel wastes: A green chemistry approach

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Citrus sector is one of the fastest growing fruit industries, owing to increased citrus production in response to rising consumer demand, generating large amounts of residues. The disposal of these wastes is considered economically and environmentally problematic if not properly converted into environmentally friendly value-added products. When properly exploited, citrus residues have economic value, since it contains plenty of interest compounds, such as pectin, flavonoids (such as hesperidin), phenolic acids, essential oils, dietary fibers, terpenoids and others. Hesperidin is the most abundant glycosylated flavanone found in citrus fruits, particularly in sweet orange albedos. Hesperidin has recently been studied for its biomedical applications; however, extraction has proven difficult due to its insolubility in water. Furthermore, the majority of the methods reported are non-selective for this flavonoid and, consequently, contribute for the presence of impurities. Pectin is a defined group of polysaccharides and one of the main components of citrus peels. The functional properties of pectin are determined by the degree of esterification, that can be classified as low methoxyl and high methoxyl pectin. Different degrees of esterification result in different physicochemical properties and applications. The yield and quality of pectin are primarily determined by the source as well as the method of extraction. The present work focused on the development and optimization of a green approach to a sequential extraction of pectin and hesperidin, while simultaneously maximizing the reuse of orange waste and solvents used. Pectin extraction was performed in acidified hot water with HCl at 0.1 M, followed by precipitation with ethanol and purification with acetone. The obtained pectin yields ranged between 17% and 19%. Hesperidin extraction was carried out in the pectin extraction residue, and an ethanolic extraction was performed with an alkaline pH (between 9 and 10) maintained throughout extraction by adding 1 M NaOH. This was followed by a 0.25 M HCl neutralization step. Furthermore, the subsequent controlled evaporation of ethanol in the rotary evaporator allowed for the immediate precipitation of hesperidin. The influence of the temperature, time and ratio of extraction have been studied with yields ranging between 0.28% and 1%. The ethanol and acetone used throughout the work were recovered and reintroduced in the sequential extraction system.

Acknowledgments: This work was supported by FCT through the CQM Base Fund - UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020, and by ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação, through the project M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM+(Madeira 14-20 Program) and project MACBIOPEST (Verónica Pereira is the recipient of a research grant - BI/MACBIOPEST/2021). Onofre Figueira is the recipient of a FCT PhD Grant in the 2021 call 2021.06250.BD.





[0-12]

Synthesis of linear dendritic block copolymers based on bis-MPA with bone targeting capability for osteosarcoma treatment

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Osteosarcoma (OS) is the most frequent primary bone tumour that mainly affects children and adolescents. Little progress for its treatment has been made in the past decades, and thus its survival rate remains below 60%, being even lower, below 20%, in the event of recurrence or metastatic disease. Cisplatin is one of the most prescribed drugs for osteosarcoma chemotherapeutic treatment, most often in combination regiment with other drugs. However, these regimens exhibit poor drug selectivity, severe adverse side effects, tumour recurrence, and some degree of permanent disability in a considerable portion of patients [1].

In this work, two novel families of dendritic-linear-dendritic (DLD) block copolymers were prepared aimed at the targeting delivery of cisplatin for osteosarcoma treatment. The DLDs were based on a hydrophilic polyethylene glycol (PEG) chain and two hydrophobic bis-MPA dendrons. The use of dendrons in the constructs will allow the adequate level of multivalency needed for interaction with the biological target and the transport of the drug. PEG will confer the system flexibility the right hydrophilicity. Here, the periphery of the DLD was first functionalized with phosphonic acid groups (DLD-phosphonic), which will provide the bone targeting capacities to the DLD, in a two-step process involving a DLD-phosphonate intermediate, followed by its deprotection. To act as a non-targeted control, a DLD functionalized with carboxylic groups (DLD-COOH) was also synthesized. Work on the functionalization of both types of constructs with cisplatin is in progress. The systems were characterized by nuclear magnetic resonance (NMR), mass spectrometry (MALDI-TOF), scanning electron microscopy coupled to Energy Dispersive X-Ray Analysis (SEM/EDX), infrared spectroscopy (FT-IR), size exclusion chromatography (SEC) and dynamic light scattering (DLS).

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Acknowledgements: This work was supported by FCT - Fundação para a Ciência e a Tecnologia through the CQM Base Fund - UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020. FM also acknowledges FCT for the PhD Grant (ref. 2021.05938.BD) and the COST action CA17140 "Cancer Nanomedicine from the Bench to the Bedside", supported by COST (European Cooperation in Science and Technology), for the STSM grant provided.

[0-13]

Discards from legumes as bacteria cryoprotectants

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The use of microorganisms, such as lactic acid bacteria (LAB), entails several benefits for certain productive sectors. However, these bacteria may undergo deterioration and loss of viability during storage. Application of galacto-oligosaccharides (GOS) can help to reduce bacterial spoilage by protecting bacteria during conservation processes such as freezing and lyophilization. Legumes contain GOS that are removed by soaking and cooking treatments applied before consumption. In this work we evaluated the cryoprotective effect of extracts obtained by processing legumes, using domestic methods, on LAB.

GOS-rich waters from chickpeas (*Cicer arietinum* L.) and lentils (*Lens culinaris* M.) were obtained by soaking (8 h, 25°C); soaking & cooking (30 min – boiling T); and cooking (30 min – boiling T) without soaking. These extracts were screened for saccharides' determination using High Pressure Liquid Chromatography with Refractive Index detection and then lyophilized. To evaluate the cryoprotective potential of the extracts, *Lactiplantibacillus plantarum* CIDCA 83114 (LP114) was added to de Man, Rogosa, and Sharpe (MRS) medium without glucose, supplemented with sugars at 3% (extracts or standards), and incubated (37° C, 24 h). After incubation, plate counts were performed on MRS agar, and the samples were divided in two groups: one was left in the freezer (-20 °C); the other was frozen, lyophilized and stored in a desiccator. Viability of LAB was evaluated immediately after freezing or lyophilization, and after two weeks in storage.

Bacterial viability diminished after applying cryoprotection processes in all samples, however when chickpea or lentil extracts were included, this effect was less intense. During storage after freezing, the extracts obtained from the soaking & cooking processes provided greater cryoprotection than those obtained using other treatments. After lyophilization, the extracts from cooking legumes without soaking showed greater cryoprotective power. Results suggest wastewaters from industrial preparation of legumes can be valuable sources of compounds with interesting potential for the cryoprotection of LAB, with great economic impact.

Acknowledgments: We thank the PREMIUM project (Preservation of microorganisms by understanding the protective mechanisms of oligosaccharides), through the European Union's Horizon 2020 grant No.777657. This work was also supported by Fundação para a Ciência e Tecnologia (FCT) through the CQM Base Fund – UIDB/00674/2020, Programmatic Fund – UIDP/00674/2020, and GNM's PhD studentship – UI/BD/152066/2021; and by Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) through ADC's PhD scholarship. Agencia Nacional de Promoción Científica y Tecnológica (ANPCyT) also funded this work [PIC (2017)/1344 and PICT (2020)/0482 projects].









[0-14]

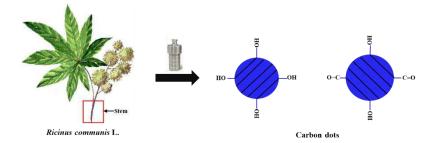
Synthesis and characterization of fluorescent carbon dots from *Ricinus communis* L.

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Invasive plants are causing a negative environmental impact, particularly *Ricinus communis* L. (RC), in the Macaronesia archipelagos. By transforming them into functional nanomaterials like carbon dots, we can contribute to the reduction of the area affected by these invasive species. Carbon dots (CDs) are fluorescent nanoparticles between 2-20 nm, discovered in 2004 by Xu and Scrivens [1]. They are photoluminescent, water-soluble, low cytotoxic, and can be surface functionalized [2,3]. CDs can be prepared by "bottom-up" methods like hydrothermal synthesis using small carbon-rich molecules or natural products (like fruits and plants) as starting materials [4]. Therefore, in this work, the main results on the use of *Ricinus communis* L. as a natural starting material for the synthesis of fluorescent CDs, will be presented and discussed. The synthesis was made using a systematic approach to study the influence on the reaction and quantum yields, and on the remaining photoluminescent properties. After synthesis, using the hydrothermal method, the carbon dots were subjected to purification and characterization using UV-Vis, fluorescence, and IR spectroscopies, DLS, as well as TEM.

Hydrothermal synthesis of carbon dots.



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Acknowledgments: The authors acknowledge FCT-Fundação para a Ciência e a Tecnologia (through Base Fund UIDB/00674/2020 and Programmatic Fund UIDP/00674/2020, Portuguese Government Funds) and the Programa de Cooperación Territorial INTERREG Iv2Mac project (MAC/4.6d/229). Filipa Pita acknowledges the financial support of Direção Regional de Juventude through the program Ingress@, and of Instituto de Emprego da Madeira through the program EPAP-Estágios Profissionais para a Administração Pública with the reference 2022/EPAP/1777.





[0-16]

Spheroid development for *in vitro* chondrogenesis – Preliminary studies

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The diseases that affect articular cartilage are a huge healthcare problem that needs to be addressed with new and more efficient treatment approaches [1]. Having this in mind, research on spheroids (a type of 3D cell aggregates aimed at mimicking biological tissues) has recently been very active as treatment solutions based on these constructs are very promising [2]. Here, three different static techniques for spheroid preparation using human mesenchymal stem cells (hMSCs) were studied. The preparation of spheroids by cell self-aggregation in ultra-low adhesion (ULA) cell culture plates was shown to be easy to use, and to lead to stable spheroids. The addition of carboxymethyl cellulose (CMC) to the basal medium (BM) contributed to control spheroid's size and spheroidicity, enhancing cell viability too. Different culture medium compositions influence on cell metabolic activity and on cell differentiation towards the chondrogenic lineage was evaluated in 2D assays. The presence of TGF-^β1, as well as other supplements to the chondrogenic medium (CM) increased cell proliferation, and induced chondrogenesis, as revealed through histochemical staining. For the assessment of the chondrogenesis in 3D constructs, spheroids were initially prepared and matured for 14 days. After this maturation period, a 28-day period of chondrogenic differentiation took place. The CM led to spheroid differentiation towards the chondrogenic lineage as an ECM of chondrogenic nature was detected by histochemical staining of the proteoglycans (chondrospheres were then obtained). Through SEM analyses it was possible to verify that the chondrospheres were more robust than the control group of spheroids kept in BM. This higher stress resistance proved to be consistent with the expected endurance associated with cartilaginous tissue. In addition to the qualitative chondrogenic potential evaluation of the generated chondrospheres, the ELISA assays allowed to detect two of the most relevant chondrogenesis markers in the chondrospheres: collagen type II and aggrecan.

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Acknowledgements: This work was supported by FCT-Fundação para a Ciência e a Tecnologia through the CQM Base Fund - UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020, and by ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação, through the project M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM+(Madeira 14-20 Program).





[0-17]

Oxidation of fluorinated PAMAM dendrimer – A combination of fluorescence and NMR traceability

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Traceable vectors that can deliver drugs or genes in a specific location are highly desirable since we can bind diagnosis and treatment in a single step. Several methods can be used to detect such vectors and nuclear magnetic resonance (NMR), as well as fluorescence spectroscopy, are two of the detection methods studied in this work. Using the generation four poli(amido) amine dendrimer (PAMAMG₄-NH₂) conjugated with 2,3,5,6-tetrafluoro-4-hydroxybenzoic acid (TFHBA) and oxidizing the resulting conjugate, we aimed to take advantage of the non-traditional intrinsic luminescence (NTIL) [1] of the PAMAM dendrimer and the fluorine to create a vector with an increased fluorescence, and that can be detected by ¹⁹F NMR [2].

Different ratios of the conjugates were synthesized, characterized, calculated their functionalization degree by NMR, and their cytotoxicity and transfection efficiency assessed. The conjugate with the better cell viability and transfection efficiency was chosen to be oxidized. The oxidation was performed based on previous work from Camacho *et al.* [3] using a range of three ammonium persulfate (APS) concentrations. The resulting was placed under a UV lamp to evaluate their fluorescence and characterized by NMR, UV/Visible, and photoluminescence. These characterizations are still ongoing. Other characterization techniques, such as Fourier-transform infrared (FTIR), Dynamic light scattering/zeta potential (DLS/ZP), and cytotoxicity and transfection efficiency studies, are to be performed. Nevertheless, strong blue fluorescence can be seen on the oxidized compounds when placed under the UV light at 366nm with fluorescence intensity differences with the increase of APS concentration.

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[0-18]

NOVAearth: A solution to wash the hands which will reduce plastic and use agri-food waste

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Responding to a more sustainable and circular economy, NOVAearth aims to create an innovative hand washing solution that can mitigate the widespread plastic problem and that uses naturally derived ingredients extracted from agri-food waste as much as possible, allowing a biodegradable formula.

The project focuses on soap refills in a concentrated powder format (biodegradable/recyclable sachets, for example, paper) that, after being diluted, produce foam instead of gel through the dispenser (Fig. 1). The reduced size and weight of this option can reduce the consumption of millions of plastic containers and both the costs and emissions associated with transporting/storing millions of liters of water (the main component of liquid soaps, 70-80%).



Fig. 1: Scheme of the concept for liquid soap refills from soluble powder, considering a B2C model (E-commerce and Supermarkets). A large container would replace the sachets in a B2B model (hotels).

In a 3-month time span, a prove-of-concept prototype was created using, at this stage, the following waste: eucalyptus leaves (invading species), orange peels (UMa bar), wood sawdust (lumber mill), used cooking oil (Tecnopolo bar). Meanwhile, avocado, and grape seed oils were bought in the supermarket instead of looking for spoiled fruit and waiting for the winemaking season, respectively, and extracting the oil ourselves.

Acknowledgments: The execution of this project was possible with the funding from the startNOW -Madeira Acceleration Program, under the research and development contract with CQM: 22-01-CQM-NE.





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Events 2021/22



















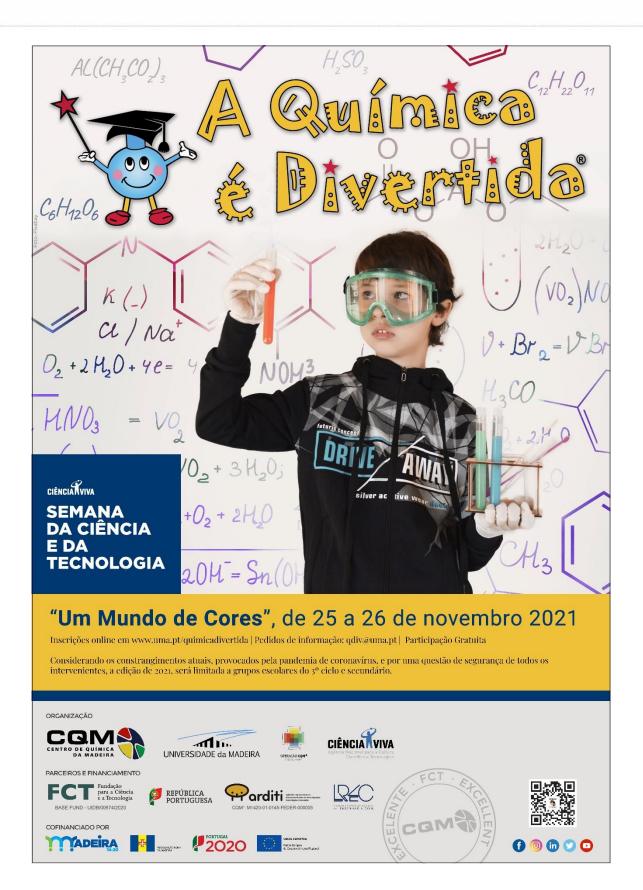
















Events 2022 (ongoing)













27th May 2022 CONFERENCE

"The Flavor Chemistry of Fortified Wines"

[A Química dos Sabores de Vinhos Fortificados]



Prof. Matteo Bordiga Food Chemistry, Biotechnology and Nutrition Unit Università del Piemonte Orientale "A. Avogadro", Italy

Conference room 0.57, 10h00 University of Madeira, Campus of Penteada

GM

PÚBLICA DRTUGUESA

14/24 PORTUGAL

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> Ferdo Europeia de Deservoiximonto Registro

N4

Registration at cqm.uma.pt [until 26th May 2022]

UNIVERSIDADE da MADEI

RCANIZATION



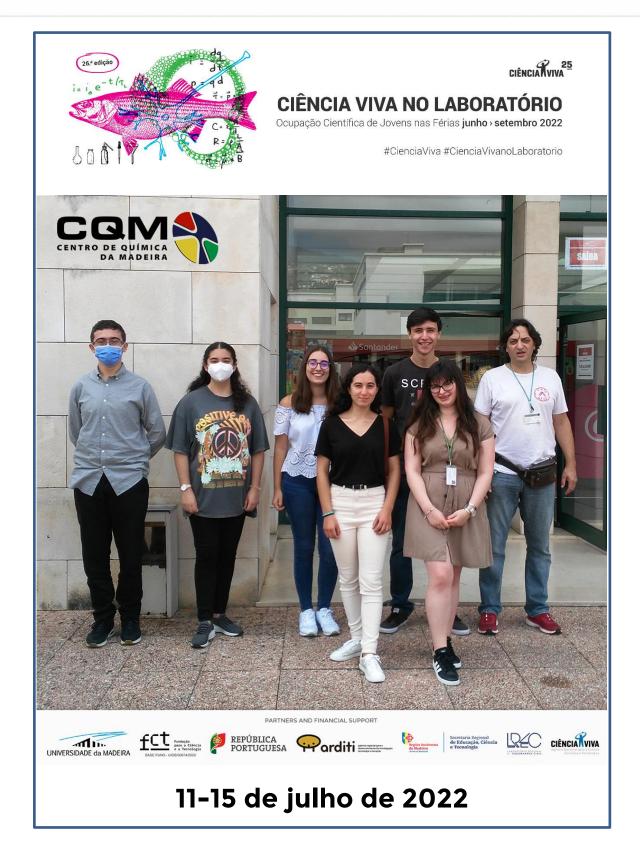




















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