8TH CQM ANNUAL MEETING

7-8 OCTOBER 2021

COLÉGIO DOS JESUÍTAS

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ABSTRACT BOOK

CQM
CENTRO DE QUÍMICA DA MADEIRA

UNIVERSIDADE da MADEIRA

8th CQM Annual Meeting

Abstract Book

7-8 October 2021

Funchal, Madeira Island – PORTUGAL

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Edited by:

João Rodrigues
Rosa Perestrelo
Énio Freitas

Organizing Committee and Secretariat:

Rosa Perestrelo
Énio Freitas
Yessyka Oliveira
Dina Maciel

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About CQM

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

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)*
Yessyka Oliveira	*Board Assistant (CQM$^+$)*
Paula Andrade	*Administrative and Technical Staff (UMa)*
Mª Teresa Abreu	*Technical Staff (CQM$^+$)*

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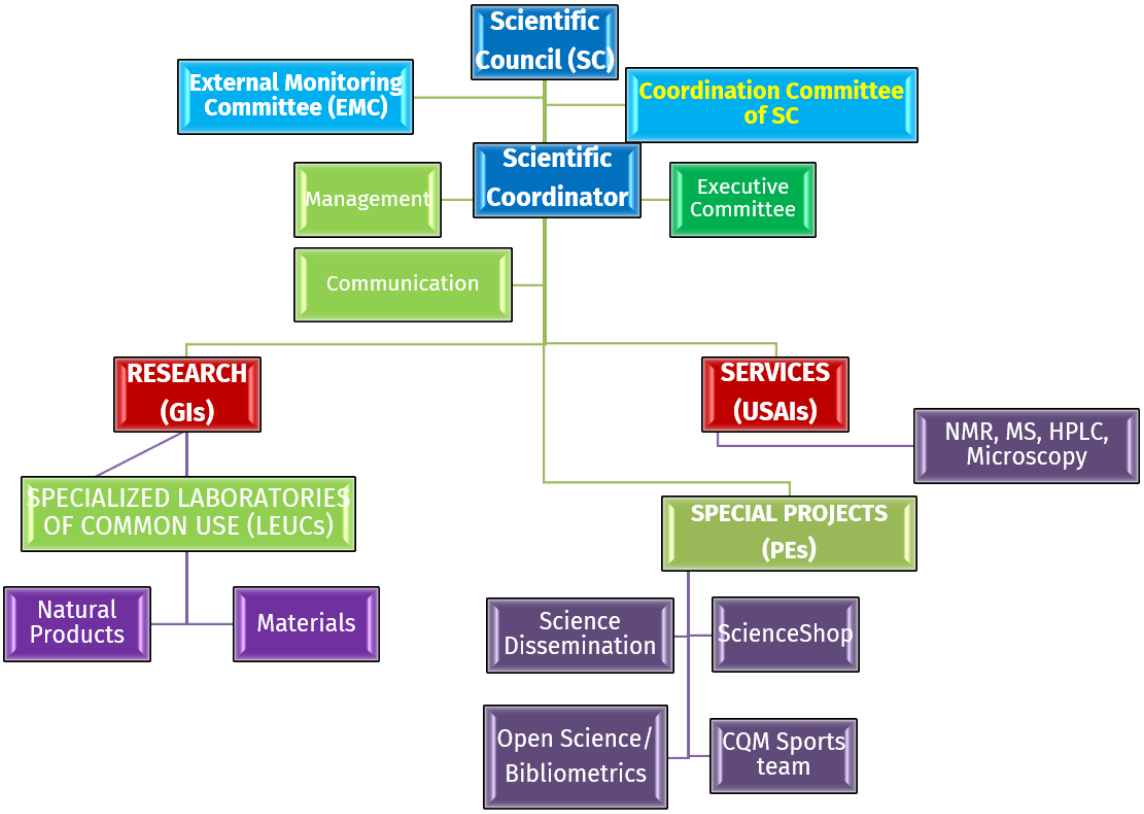
Makoto Fujita	*Full Professor, Department of Applied Chemistry, University of Tokyo, Japan*
John Beutler	*National Cancer Institute – Center for Cancer Research, USA*
Jean-Pierre Sauvage (2016 Nobel Prize in Chemistry)	*Institut de Science et d'Ingénierie Supramoléculaires, University of Strasbourg (France).*

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 - An endless journey

More than 15 years after CQM launching (CQM was created in 2004 as a Foundation for Science and Technology Centre - FCT Centre), the main objective of the founders, a handful of Ph.D. researchers from the Chemistry Department of the University of Madeira (UMa) was achieved. In 2021, CQM obtains, for the first time, in the scope of the international evaluation process of the Portuguese research units carried out by FCT, the highest classification possible to be obtained by a Research Centre in Portugal - **EXCELLENT**. If for some inside and outside the University of Madeira (and even for some belonging to the Centre itself), this was something they thought would never be possible, for those who knew our work, commitment, and organizational capacity, it was clear that, sooner or later, this objective would be achieved.

- For the first time, CQM was evaluated with the highest classification possible to be obtained by a Research Centre in Portugal.

In fact, the work carried out by the Centre, and its impact on the Region is proof that investment in research units, even of small size and without economy of scale, but with highly motivated, organized teams with an international vision, are worth it. These can generate highly qualified employment, enhance the production of knowledge with an economic impact, give international visibility to the regions and the country and even respond to emergencies like the one that has affected the world in the last two years. However, to get here, in addition to hard work and strong conviction, it was necessary to overcome not only the prejudice of size and geographic location but also the many difficulties that daily arise to a centre located in a region where the areas of political/scientific interest were not always coincident with its pathway. To these difficulties, CQM members have always responded with resilience and ambition. Indeed, CQM's human capital is today as tomorrow, our asset, our great strength. It was our choice to believe that it was possible to build something from scratch, even if we had to learn and make mistakes countless times, work with few resources, and in a small, new, and naturally peripheral institution. This is our victory, a victory of the University of Madeira and the Autonomous Region of Madeira!

- CQM team during the 7th Metting in 2020.

In these 17 years of CQM existence, the impact of our work is reflected in the indicators of scientific production, dissemination of science, services to the community, and the scientific support given to courses led by the Chemistry Department. Indeed, without locally trained human resources, not only would we not have been able to be internationally competitive, but it would also be impossible to respond to the Region's needs in terms of highly qualified human resources. If there are doubts about this last aspect, one should pay attention to the level of employability in times of pandemic of the human resources formed by the Chemistry Department and by us.

Here are some figures of the work done. From 2004 until 2020, the CQM published:

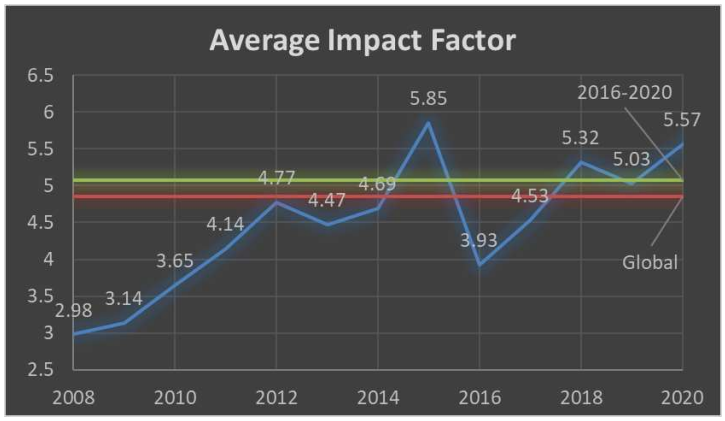
- **492** papers with impact factor:
  - An average of 1.28 papers/researcher/year or 31 papers with IF per year.
- **12** papers without impact factor
- **19** books and book chapters
- **13** Proceedings
- **60** doctoral (D) and master (M) theses:
  - **14**(D) and **46**(M)

  - **TOTAL OF PUBLICATIONS** (2004 to 2020): **616**
    - or 38.5 publications/year

In **2020/2021** (provisional values) the Center published as follows:

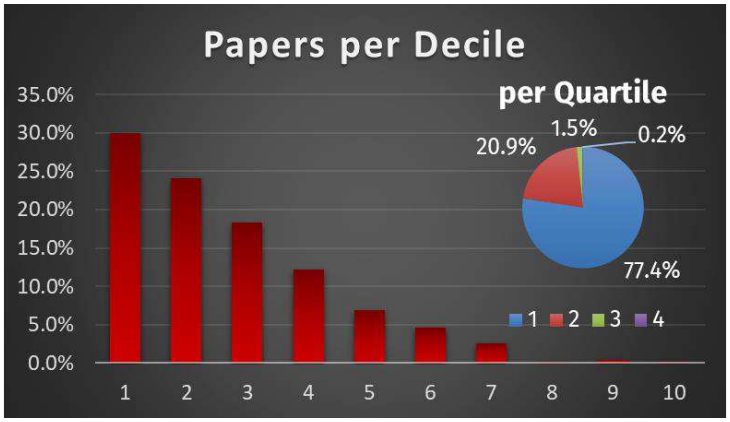
- Papers with impact factor: **113** (73/40)
  - Average of papers published in 2020: **3** papers/researcher
- Papers without impact factor: 3/1
- Books and book chapters: 1/-
- Doctoral (D) and Masters (M) theses: **7** (1/1(D) and 3/2(M))
  - **TOTAL OF PUBLICATIONS** (2020/2021): **125** (81/44)

Given the number of publications with impact factors, it is important to look for their scientific relevance, analysing at the 2008-2020 period, respectively, the average impact factor (AIF), the distribution of these publications by deciles and quartiles of journals, and the accumulated number of citations (total of citations). In a first analysis, there is a growing trajectory in the AIF of CQM papers with time. With the AIF value reaching its maximum (5.85) in 2015 with 35 published papers. Year in which the CQM published in *Chemical Reviews* and *Progress in Polymer Science*, journals that, due to their characteristics, mainly publishing review articles, have very high impact factors.



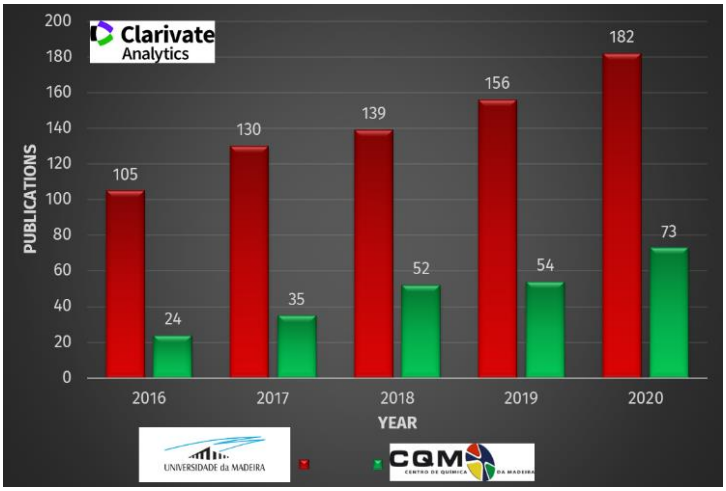
- Average impact factor (AIF) in 2008-2020 period.

As for the distribution of publications by quartiles and deciles for the period 2008-2020, it is noted that 77.4% of the publications were made in journals in the 1st quartile and, even though 30% or 142 papers were published in 1st decile journals.



- CQM papers distribution by deciles and quartiles in 2008-2020 period.

Regarding the accumulated number of citations, in 2020 its value reaches 16294 citations or 33 citations per published paper. It can be concluded from the above that CQM researchers, in the period under review, have not only published in a remarkable way for the size of the unit, as their work was highly cited and published in journals of high scientific impact. Analysing the AIF data on a more recent period (2016 to 2020), the AIF values remained mostly above 5 and reached, in 2020, the second-highest value ever in terms of average impact factor (5.57).



- CQM Publications 2016-2020.

Results that consolidate the evolutionary trajectory of CQM and, concerning the year 2020, are particularly remarkable considering the current pandemic moment. In fact, despite the CQM's laboratory activity having been partially interrupted in 2020, we managed not only to reach the highest number of articles with IF, published in a single year (73), as we also had the organizational capacity to support the Region, through the Service of RAM (SESARAM), in the production of an alcoholic-based antiseptic solution (ABAS). Specifically, in the three campaigns carried out by CQM, from April 9, 2020, to October 30, 2021, were produced and delivered to SESARAM, 8310 Liters of ABAS.

- Alcoholic-based antiseptic solution (ABAS) produced by CQM during the pandemic.

Moreover, if the CQM has not registered any patent in the Region, this is due to several factors. For example, the nature of the produced knowledge, the absence of human resources at CQM/UMa specifically devoted to patent development, and, of course, the cost of maintaining these patents. Still, we have maintained a close collaboration with companies from and outside the Region, e.g., consultancy, service

provision, and training of highly qualified staff (who currently occupy prominent positions at private and public companies). This is an important economic impact, but one is difficult to account. For sure, the time for patents in CQM/UMa will naturally come without the pressure of numbers and statistics.

Furthermore, if publications are an essential milestone for any research center, the financial support achieved by the CQM during this period is remarkable. Thus, from 2004 to 2020, CQM managed a financing portfolio worth more than 11.4 million euros. This financing will be reflected in coming years, namely with the acquisition and installation of various equipment, such as the liquid nitrogen production unit, which will be installed in the following weeks, and which it will represent for the CQM and the Region, thanks to the funds of Madeira 14-20 Program, an investment of more than 120,000 euros.

- Illustration of the liquid nitrogen production unit to be installed by CQM.

Having arrived here, the CQM must continue to work to repeat the achieved classification in the next evaluation. However, if it is true that much depends on us, another part already ultimately transcends us. Maintaining this assessment will certainly be more difficult than conquering it for the first time.

To keep serving the country and the Region, regular funding should be ensured that will allow us to recruit the best human resources and maintain the best-trained and innovative researchers who make up the CQM team today. Effectively, a research centre that wants to be internationally competitive must have a permanent team of researchers, research technicians, and a minimum administrative staff, with higher education, to ensure normal functioning. In fact, we do not foresee it being possible to maintain the level of assessment achieved and contribute to the national and regional smart specialization strategy without:

a) A stable team of 20-25 PhDs (with employment contracts and research grants);
b) A technical/administrative and permanent communication and dissemination team;
c) Investing in the renovation of spaces and equipment;

d) Continuing to have the capacity to attract highly qualified human resources in the international market that will complement the existing critical mass and can bring scientific and financial added value to the CQM and the Region.

In addition, together with careful management of the funds at our disposal, and organizational philosophy that strives to reduce as much as possible the time spent by researchers on tasks other than those related to their research work, we must remember that to remain competitive, it is necessary to go beyond what we are doing today. Whether looking shortly for skills in the areas of artificial intelligence, big data, and robotics (aspects already placed under consideration the consideration of the Regional Government), or by storing, protecting, curating, and validating data, producing new data, and making them available to the scientific community. Recent experience shows us that storage, curating, and availability of data in a network constitutes a financial asset and contributes to a faster and more effective resolution of problems.

Once the pandemic is over, the future of academic institutions and regions cannot be made without a regular investment in research centres of excellence, funding which cannot be exclusively dependent on the FCT or inconstant European Projects. To achieve the CQM team's hope, it is time to materialize the wishes and respond, with decisions, to the identified problems. The CQM, as a small research unit, will continue to fulfil its mission, always at the service of the University, Region, and Country.

University of Madeira, Funchal, 6th of October 2021

(João Rodrigues, Scientific Coordinator of CQM)

Program

Thursday, 7th October 2021		
09:30	10:15	**Opening Session** Professor Sílvio Fernandes *Rector of the University of Madeira* Dr. Miguel Albuquerque *President of the Regional Government of Madeira* Dr. Francisco Fernandes *President of the General Council of the University of Madeira* Dr. Rui Caldeira *President of the Administration Council of ARDITI* Professor José Baptista *President of the Faculty of Exact Sciences and Engineering* Professor João Rodrigues *Scientific Coordinator of CQM*
10:15	10:45	**Coffee-break**
Chairperson: Jorge Pereira		
10:45	11:20	[O-01] **The effect of copper dopping on the morphology of magnesium oxide nanoparticles prepared via calcination facilitated sol-gel approach** Jaison Jeevanandam & João Rodrigues
11:20	11:45	[O-02] **Mechanisms of polyphenols' action against diabetes related pathologies** João Serina & Paula C. Castilho
11:45	12:10	[O-03] **Exploring new routes in the preparation of carbon dots for biomedical applications** Ivo J. Martins, Filipa Pita, Helena Tomás & João Rodrigues
12:10	12:25	[O-04] **Differentiation of roasted ground coffee by geographic origin using solid phase microextraction combined with gas chromatography-mass spectrometry and chemometrics** Carolina Andrade, Rosa Perestrelo & José S. Câmara
12:25	12:40	**8th CQM Annual Meeting - Group Photo**
12:40	14:25	**Lunch**
Chairperson: Rita Castro		
14:25	15:00	[O-05] **Ligand development by phage display technology – Application to bionanosensors for the diagnosis of Zika** Mariana Vieira, Helena Chá-Chá, Helena Caldeira, Helena Tomás & João Rodrigues

15:00	15:25	[O-06] **Extraction and characterization of bioactive compounds from selected Macaronesia plants as sources of biopesticides** Rui Ferreira, Iria López, Vanessa Santos & Paula C. Castilho
15:25	15:50	[O-07] **Bisphosphonates: a brief review and envisaged work towards osteosarcoma treatment** Fátima Mendes, Filipe Olim, Ana Rute Neves, João Rodrigues & Helena Tomás
15:50	16:15	[O-08] **Pepsinogen from *Aphanopus* spp. and *Thunnus obesus* immobilization in chitosan spheres** Pedro Ideia, Onofre Figueira & Paula Castilho
16:15	16:30	[O-09] **The synthesis of Cu DENPs using ascorbic acid and hydrazine as reducing agents** Duarte Fernandes, Mariana Vieira, Carla S. Alves, João Rodrigues & Pedro Pires

Friday, 8th October 2021		
Chairperson: Mara Gonçalves		
09:00	09:35	[O-010] **Preparation of Gemcitabine and cisplatin-modified PAMAM dendrimer aiming its stimuli-responsive co-delivery towards pancreatic cancer** Rita Castro, Helena Tomás & João Rodrigues
09:35	10:00	[O-011] **Molecular identification of *Saccharomyces cerevisiae* strains from Madeira Island** Mariangie M. Castillo, José S. Câmara & Mahnaz Khadem
10:00	10:15	[O-012] **A fluorinated dendrimer for traceable gene delivery** Lydia dos Orfaos, Helena Tomás & João Rodrigues
10:15	10:40	[O-013] **Polyphenolic profile, antioxidant and anti-diabetic potential of berries-producing plants after in vitro gastrointestinal digestion** Joana Pinto, Vitor Spínola & Paula C. Castilho
10:40	10:55	[O-014] **Hyperhomocysteinemia and oxidative stress in vascular disease: Evalution of glucose-6-phospahte dehydrogenase in HUVEC cells** Isabel Faria, Mariana Vieira, Celso Cunha & Helena Caldeira
10:55	11:25	**Coffee-break**
Chairperson: Mariana Vieira		
11:25	11:50	[O-015] **Immobilization of β-galactosidase in calcium alginate beads** Gonçalo Nuno Martins, Onofre Figueira & Paula C. Castilho

11:50	12:15	[O-016] **Establishment of urinary volatomic profiles for the identification of putative prostate cancer biomarkers** Cristina Berenguer, Ferdinando Pereira, Ricardo Sousa, Jorge A.M. Pereira & José S. Câmara
12:15	12:30	[O-017] **Induction of the osteogenic differentiation of human Mesenchymal Stem Cells by Protamine/pDNA/PAMAM-COOH ternary complexes** Fátima Moreira, Filipe Olim, Helena Tomás & Rita Castro
12:30	13:00	**Closing session**

Oral Communications

[O-01]

The effect of copper dopping on the morphology of magnesium oxide nanoparticles prepared via calcination facilitated sol-gel approach

Jaison Jeevanandam[1] & João Rodrigues[1,2*]

*[1]CQM-Centro de Química da Madeira, MMRG, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal. *joaor@uma.pt*
[2]School of Materials Science and Engineering, Center for Nano Energy Materials, Northwestern Polytechnical University, Xi'an, 710072, China.

Magnesium (Mg^{2+}) ions act as a co-factor for more than 300 enzymes and trigger processes such as the synthesis of RNA and stimulation of hormones [1]. In general, magnesium hydroxide ($Mg(OH)_2$), magnesium peroxide (MgO_2), and magnesium oxide (MgO) are the common sources of magnesium ions. Nevertheless, the high mechanical stability with enhanced physicochemical properties of MgO, such as low toxicity, high bioavailability, high thermal conductivity, and stability, makes them a superior source of Mg^{2+} ions, compared to other magnesium-based compounds. Further, these MgO in its nanoform is identified to be beneficial for biomedical applications due to their superior biosorption, solubility and bioavailability, stable thermodynamics, and physicochemical properties [2]. Furthermore, it is noteworthy that the synthesis approach plays a major role in determining the properties of MgO nanoparticles. Physical methods such as laser ablation, radiofrequency sputtering, and chemical approaches such as co-precipitation, hydrothermal, sol-gel, and solvothermal are the conventional synthesis methods used to synthesize MgO nanoparticles. However, physical methods are not suitable for large-scale nanoparticle synthesis of metallic oxides due to the involvement of expensive equipment and high energy sources. Among various chemical processes, the sol-gel technique is simple, requires low reaction temperature, is cost-effective, and yields smaller MgO nanoparticles with a high surface area to volume ratio. However, achieving desired smaller-sized MgO with a specific shape, monodispersity, and high stability is still a challenge in the sol-gel approach [3].

The doping of the MgO crystal lattice structure with metal ions has been proven to create defects to modify their physicochemical properties and the morphology of the MgO nanoparticles [4]. Thus, we aim to prepare MgO nanoparticles via sol-gel approach in the present work and identify the effect of metal dopant (copper), dopant precursor (copper acetate and copper nitrate) and concentration (1, 2, and 3%), calcination time (2, 3 and 4 h) and temperature (550, 650 and 750°C) on the morphology of the resultant nanoparticle. The systematic characterization showed that the dopant source and concentration affect the nanoparticles' size (~30-70 nm), whereas the calcination time and temperature influence its morphology by transforming them from spherical to hexagon and from hexagon to elongated hexagon.

References: [1] K Pasternak, J Kocot, A Horecka, *J. Elem.* **2010**, 15: 601. [2] ST Khan, AA Al-Khedhairy, **2017**. Metals and Metal Oxides: Important nanomaterials with antimicrobial activity. In *Antimicrobial Nanoarchitectonics* (pp. 195-222). Elsevier. [3] JP Singh, V Singh, A Sharma, G Pandey, KH Chae, S Lee, *Heliyon* **2020**, *6*: e04882. [4] V Rajendran, B Deepa, R Mekala, *Mater. Today: Proc.* **2018**, *5*: 8796.

Acknowledgments: The authors acknowledge the support of FCT-Fundação para a Ciência e a Tecnologia (Base Fund UIDB/00674/2020 and Programmatic Fund UIDP/00674/2020, Portuguese Government Funds), ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação through the project M1420-01-0145-FEDER-000005-CQM+ (Madeira 14-20 Program).

[O-02]

Mechanisms of polyphenols' action against diabetes related pathologies

João Serina & Paula C. Castilho

CQM – Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal.

Diabetes incidence has been considerably rising in the past decades and this behaviour is projected to continue in the coming ones. Affecting an estimated 463 million people worldwide in 2019, this metabolic disorder can be caused by several factors and will lead to devastating complications that severely damage the patient's health and greatly diminish their quality of life. Polyphenols, mostly in the form of plants and extracts, have long been used in popular and traditional medicine to treat or reduce the progression of diabetes and its complications. By analysing the many categories of polyphenols and their effects in diabetes, patterns start to emerge, and five key mechanisms / actions become apparent: mimicking of caloric restriction, increased uptake and use of glucose, anti-inflammatory effect, antioxidant effect and genetic regulation. In this work we will approach each of these effects in the context of diabetes and how polyphenols can contribute to the future of diabetes therapy.

Acknowledgments: The authors acknowledge the support of FCT-Fundação para a Ciência e a Tecnologia (Base Fund UIDB/00674/2020 and Programmatic Fund UIDP/00674/2020, Portuguese Government Funds), ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação through the project M1420-01-0145-FEDER-000005-CQM+ (Madeira 14-20 Program). João Serina would also like to acknowledge FCT - Fundação para a Ciência e a Tecnologia for the PhD grant 2020.05328.bd.

[O-03]

Exploring new routes in the preparation of carbon dots for biomedical applications

Ivo J. Martins, Filipa Pita, Helena Tomás & João Rodrigues*

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

Developing new and innovative nanomaterials is essential to progress nanotechnology, and in this regard, carbon-based nanomaterials are among the most explored by the scientific community. Carbon dots (CDs), one of the most recent types of carbon-based nanomaterials, consist of quasi-spherical nanosized particles (<10 nm) composed internally by carbon sp^2/sp^3, and the surface by different functional groups like carboxyl or amide, turning them photoluminescent, water-soluble and low cytotoxic [1,2]. CDs can be prepared by bottom-up methods like hydrothermal or microwave synthesis, using carbon-rich starting materials commonly found on our lab shelves or from natural sources [3]. Their ability to interact by π-π stacking, hydrogen, and covalent bonding, allows their combination with various chemical structures, drugs, or genetic material making them strong candidates for biomedical applications [4].

In this work, carboxyl-CDs were prepared using hydrothermal approach and ascorbic acid as starting precursor and further characterized by UV-Vis, Fluorescence, IR, and NMR spectroscopies, as well as TEM, AFM, and DLS. Then, the prepared CDs with anionic surface were combined with G4-G6 PAMAM-NH_2 dendrimers to form G4-G6 CDs@PAMAM nanohybrids, and their potential for bioimaging and gene delivery was studied [5]. Furthermore, the carboxyl-CDs were surface-functionalized with 4-aminobenzonitrile to enhance its photoluminescent properties and complex with $RuCl(PPh_3)_3(C_5H_5)$, forming Metallo-CDs. Lastly, invasive plants from the Macaronesia archipelagos were explored as a new carbon source for the synthesis of fluorescent carbon dots. All these promising results will be presented and discussed, having in view their potential biomedical applications.

References: [1] O Kozák, M Sudolská, G Pramanik, P Cígler, M Otyepka, R Zboril, *Chem. Mat.* **2016**, 28: 4085. [2] A Cayuela, ML Soriano, C Carrillo-Carrión, M Valcárcel, *Chem. Commun.* **2016**, 52: 1311. [3] G Ge, L Li, D Wang, M Chen, Z Zeng, et al., *J. Mater. Chem. B* **2021**, 9: 6553. [4] F Yan, Y Jiang, X Sun, Z Bai, Y Zhang, X Zhou, *Microchim. Acta* **2018**, 185: 424. [5] I Martins, H Tomás, F Lahoz, J Rodrigues, *Biomacromolecules* **2021**, 22: 2436.

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[O-04]

Differentiation of roasted ground coffee by geographic origin using solid phase microextraction combined with gas chromatography-mass spectrometry and chemometrics

Carolina Andrade[1], Rosa Perestrelo[1] & José S. Câmara[1,2*]

[1]CQM – Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal.
*[2]Departamento de Química, Faculdade de Ciências Exatas e Engenharia, Campus Penteada, Universidade da Madeira, 9020-105 Funchal, Portugal. *jsc@staff.uma.pt*

Coffee is a popular beverage worldwide, that is produced from the seeds of plants belonging to the *Coffea* genus. It is estimated that, during 2020, coffee production exceeded 169 million 60 kg bags, proving coffee's economic significance. Aroma is an important characteristic that influences coffee quality in addition to consumer preference. It depends on several factor, such as variety and geographic origin. The main coffee varieties with commercial relevance are *Coffea arabica* and *Coffea canephora* var. robusta. Since Arabica beans produce a sweeter, softer beverage with a better taste when compared to the stronger, harsher tasting coffee obtained from robusta beans, it is considered more valuable and, consequently, more expensive. The authentication of foods and food-derived products, namely those with high commercial value, has become of rising concern, motivating the development of high-resolution analytical tools in order to mitigate the situation.

In this context, the aim of the present work was to differentiate Arabica coffees from five distinct geographic origins (Brazil, Colombia, Ethiopia, Guatemala, and Timor) using headspace solid phase microextraction combined with gas chromatography-mass spectrometry (HS-SPME/GC-MS) and chemometric analysis. A total of 110 volatile organic compounds (VOCs) were identified in the roasted ground coffee samples - 93 in Brazilian and Ethiopian, 89 in Timorese, 87 in Colombian and 81 in Guatemalan coffees. From the different chemical families identified, furanic and nitrogen compounds were the dominant contributors to the volatile composition of all samples. Overall, higher volatile concentrations were observed in Ethiopian coffee and lower on Guatemalan coffee, while there were no significant variations among coffee from other origins. The VOCs that allowed the geographical discrimination of the coffee samples were 2,3,6-trimethyl-1,5-heptadiene, methyl-2-butanoate, β-terpinene, *o*-cymene, 2,7-dimethyloxepine, 2-methyl-5-propylpyrazine, 2-ethyl-1-hexanol, 2,3-diethyl-5-pyrazine, 2-methoxy-3-(2-methylpropyl)pyrazine and m-tert-butylphenol.

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[O-05]

Ligand development by phage display technology – Application to bionanosensors for the diagnosis of Zika

Mariana Vieira, Helena Chá-Chá, Helena Caldeira, Helena Tomás & João Rodrigues

CQM - Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal.

Zika is an infectious disease transmitted by Zika virus with no treatment or vaccine currently available. Current diagnostic tools for this disease are based on serological studies and antigen/genome detection, which are time-consuming and require expensive and specialized laboratory equipment [1]. Specificity is also a problem since cross-reactivity with other similar viruses is common and will originate false positive results. Therefore, the main purpose of this work is to overcome these challenges by developing an approach, based on phage display technology that will allow for an early, rapid and differential routine diagnosis of Zika.

The phage display technique allows for the presentation of randomized peptide sequences on the surface of bacteriophages, which can be used for the affinity screening of specific target molecules [2]. This technology consists primarily on a "panning" method, where phages bound to a specific target go through several repeated cycles in order to produce a phage mixture enriched with the phage-displayed peptides that specifically recognize target molecules with high sensitivity and selectivity. The target-bound bacteriophages and their corresponding peptides are then amplified, identified, and characterised.

In this work, a peptide library was used towards Zika-specific antibodies to identify peptides that specifically recognize those antibodies. These peptides were also screened against sera from healthy individuals and sera containing anti-Zika antibodies, in order to increase their sensitivity and specificity against their targets. This work provides new insights into the development of robust bionanosensors as sensitive diagnostic tools for Zika. The ideal outcome will be an innovative biosensing method for non-invasive, rapid, and in real time diagnosis for this infectious disease.

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[O-06]

Extraction and characterization of bioactive compounds from selected Macaronesia plants as sources of biopesticides

Rui Ferreira[1], Iria López[1,2], Vanessa Santos[1] & Paula C. Castilho[1]

[1]CQM – Centro de Química da Madeira, Campus Universitário da Penteada, 9000-390 Funchal, Portugal.
[2]Escola de Enxeñería Industrial, Universidade de Vigo, Campus Vigo Tecnolóxico, 36310 Vigo, España.

One of the guidelines for Integrated Pest Management policy is the study of new botanical biopesticides obtained from by-products from agriculture/forest management and underused plants, by evaluation of cytotoxic and phytochemical activities of plant extracts rich in secondary metabolites (flavonoids, hydroxycinnamic acids, terpenes and/or alkaloids) against pest and pathogens relevant to crops and cultures.

In this study, discards from plant trimming of endemic and introduced species from flowering genera that thrive in Macaronesia - *Helichrysum*, *Clinopodium, Cedronella* and *Origanum*, were extracted to obtain bioactive compounds. Two extraction methodologies were applied: an ultrasonic assisted extraction and a 72h agitation cycle extraction, both using organic solvents such as ethanol and hexane. Conditions were optimized, depending on plant species and solubility for each extractive. Hydrodistillation with a Clevenger-type apparatus was used for high volatile extractives, with a strong emphasis on "green technology".

The essential oils obtained by hydrodistillation were subjected to TLC with silica gel for class separation before GC-FID quantification. FTIR-ATR spectroscopy and high-resolution ^{1}H and ^{13}C NMR spectroscopy were also used for characterization of bioactive compounds.

As for extraction with organic solvents, for all species the ethanolic fraction obtained from 72 h agitation cycles produced higher yield than the ultrasonic assisted methodology. *Helichrysum* and *Origanum* extracts consist mainly of phenolic compounds and monoterpenes.

The essential oils obtained from *Helichrysum* and *Clinopodium* were dominated by monoterpene *p*-menthane derivatives: pulegone and isopulegol. Since isopulegol has 8 possible enantiomers, NMR spectroscopy was the only technique that allowed for the exact identification. Pinocarvone, a stereoisomer of carvone, was the main constituent for *Cedronella*, corroborated by IR data for this specie. *Origanum* vulgare EO is characterized for its high content in carvacrol, thymol and β-caryophyllene.

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[O-07]

Bisphosphonates: a brief review and envisaged work towards osteosarcoma treatment

Fátima Mendes, Filipe Olim, Ana Rute Neves, João Rodrigues & Helena Tomás*

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

Bisphosphonates have become the standard treatment for various bone related illnesses, namely osteoporosis, Paget's disease, and *Osteogenesis Imperfecta*. In the last decades, research has focused not only on overcoming their drawbacks, such as low bioavailability and side effects, but also on their use as targeting agents for the delivery of other molecules to bone tissue for the treatment of diseases like bone cancer and metastasis [1,2]. Moreover, a few works report the use of bisphosphonates in nanomedicine, which are transported by nanocarriers as the main active compound, or as bone targeting moieties, thus making part of nanocarriers structure. In this case, bisphosphonates may enable the targeted delivery of drugs that have no special affinity to the bone tissue.

Osteosarcoma (OS) is a bone malignancy characterized by production of osteoid by bone forming cells. Its 5-year survival rate remains below 60%, decreasing below 20% in case of metastatic disease or recurrence. Currently, its first line treatment is systemic chemotherapy, consisting of a combination regimen of doxorubicin, cisplatin and methotrexate. However, it is associated with poor selectivity of the drugs, severe adverse side effects and tumour recurrence. It has been shown that OS's cells produce soluble factors (e.g., IL-6, IL-11, TNF-α, RANKL) that activates osteoclastogenesis, and thus bone degradation. In turn, growth factors released from bone matrix (e.g., IGF-1 , TGF-β), besides raising extracellular Ca^{2+} concentration, stimulate tumour growth, thus creating what is known as the "vicious cycle of the osteosarcoma" [3,4].

Herein, a brief summary of bisphosphonate types, properties, and current applications will be presented. Particularly, examples of their use in association with nanotechnology solutions for medical applications will be highlighted. Furthermore, the workplan for the future development of a drug delivery system based on biodegradable dendrimers and bisphosphonates for the treatment of osteosarcoma will be presented.

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[O-08]

Pepsinogen from *Aphanopus spp.* and *Thunnus obesus* immobilization in chitosan spheres

Pedro Ideia[1,2], Onofre Figueira[1] & Paula C. Castilho[1]

[1]CQM – Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105, Funchal, Portugal.
[2]DSEIMar – Direção de Serviços de Monitorização, Estudos e Investigação do Mar, Avenida do Mar e das Comunidades Madeirenses, 23, 9000-054, Funchal, Portugal.

Black scabbardfish (*Aphanopus spp.*) and bigeye tuna (*Thunnus obesus*) are two of the most important fish species landed in Madeira Island, representing the majority of total catches (around 80% to 85%) and consequently the majority of the revenue resulting from the fishing activity of the archipelago. Such a large number of catches implies an equally large production of wastes subsequent of the fishing industry. Viscera, that constitutes about 5% of the fish weight, is one of the most important wastes/by-products, due to the presence of digestive proteolytic enzymes. Several of these digestive enzymes, being aspartic protease pepsin one of the most important, are of great potential for human health applications. Pepsin and pepsinogen (pepsin inactive precursor), for example, are employed in several industrial applications, such as collagen extraction, medical research, cheese making, fish silage and fish processing.

In the present study, pepsinogens from viscera of *Aphanopus spp.* and *T. obesus* were extracted, partially purified by fractionating with ammonium sulphate and characterized. Pepsinogens were then immobilized onto chitosan beads aiming at re-usage, extended period of usage time, resistance to enzyme inhibitors and application as heterogeneous catalysis, while ensuring its catalytic functions. Immobilization efficiency and capacity were assessed, as well as enzymatic kinetics and inhibition towards known pepsin inhibitors, for preactivated and non-preactivated pepsinogens immobilized in chitosan spheres. The spheres were characterized by FTIR and SEM.

Results revealed a successful immobilization with high immobilization efficiency values for commercial pepsin and pepsinogens from *Aphanopus spp.* and *T. obesus* of 99%, 91% and 90%, respectively. It was also possible to verify higher immobilization capacities for the extracted pepsinogens (> 256 mg/g) than for the commercial pepsin (aprox. 34 mg/g). The immobilization material granted a protective behavior towards the pepsinogen, when immobilized in its non-preactivated form, with relative activity between 94% and 100%.

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[O-09]

The synthesis of Cu DENPs using ascorbic acid and hydrazine as reducing agents

Duarte Fernandes[1], Mariana Vieira[1], Carla S. Alves[1], João Rodrigues[1,2] & Pedro Pires[1,*]

*[1]CQM – Centro de Química da Madeira, Universidade da Madeira. Campus Universitário da Penteada, 9020-105 Funchal, Portugal. *pedro.pires@staff.uma.pt*
[2]School of Materials Science and Engineering/Center for Nano Energy Materials, Northwestern Polytechnical University, Xi'an 710072, China.

As opposed to more expensive and less earth-abundant metals like silver and gold, copper and particularly copper-based nanoparticles (CuNPs) are expected to be a more sustainable material. Also, the good physicochemical properties (e.g., electronic, optical, antimicrobial) displayed by copper materials make them attractive for industrial applications. However, CuNPs are intrinsically unstable under atmospheric conditions, making them prone to oxidation. To increase the stability of CuNPs, various efforts have been made involving, for instance, the association of CuNPs and organic compounds such as polymers [1,2].

This work aims to develop a synthesis procedure of long-term stable Cu-based dendrimer entrapped NPs (CuDENPs) and their characterization. Fourth-generation hydroxyl-terminated polyamidoamine (PAMAM) dendrimer was used as a template for the controlled growth of the Cu NPs. The ascorbic acid and hydrazine were used as reducing agents, individually or combined (hybrid route).

From the three reducing agent approaches used, only the ascorbic acid and the hybrid routes led to the formation of particles in suspension. Thus, the particles from the hydrazine route were only characterized by Scanning Electron Microscopy (SEM). Over time spectroscopic measurements (UV-Vis and fluorescence) of the prepared CuDENPs suggested considerable stability of the CuNPs. Analysis by nuclear magnetic resonance (NMR) spectroscopy indicated that the signals from the dendrimer were highly dependent on the nature of the composite, which is most likely related to the Cu oxidation state. The prepared CuNPs appear not to be cytotoxic up to 100 µg/mL concentrations by resazurin metabolic assay. Very preliminary antimicrobial activity results show no significant *E. Coli* growth inhibition, but further studies are underway to reconfirm these first. Complementary characterization is ongoing to elucidate better the final product's size, structure, and chemical nature.

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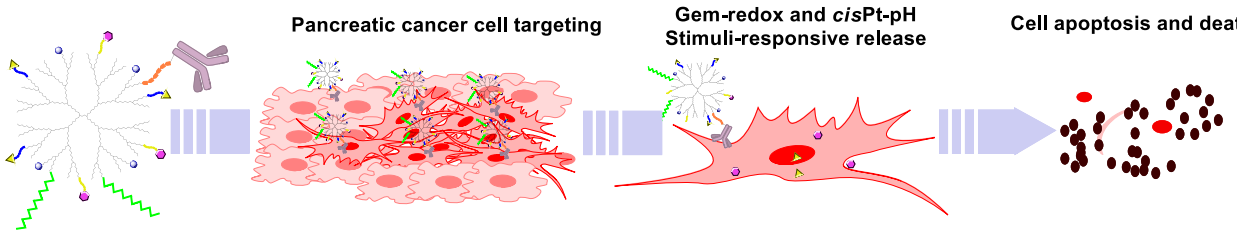
[O-10]

Preparation of Gemcitabine and cisplatin-modified PAMAM dendrimer aiming its stimuli-responsive co-delivery towards pancreatic cancer

Rita Castro, Helena Tomás & João Rodrigues*

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

Polyamidoamine (PAMAM) dendrimers, due to their physical and chemical properties, have given proof of its ability to be applied as an efficient drug and gene delivery system. For instance, its hyperbranched structure with terminal multifunctional groups, has allowed the chemical conjugation of one or several types of molecules for therapeutic and/or targeting purposes [1]. Pancreatic ductal adenocarcinoma (PDAC) is the most common pancreatic cancer type, with high mortality and low survival rate [2]. Its treatment usually requires drug combination, such as using Gemcitabine (GEM) and cisplatin (*cis*Pt) to overcome drug resistance [3]. Here we propose using PAMAM dendrimers to co-deliver, in a pH and redox-stimuli responsive manner, both GEM and *cis*Pt, aspiring an enhanced efficacy and lower doses potentially leading to reduced side effects [4]. Initial generation 5 (G5) PAMAM dendrimer terminal groups modification was successfully performed, namely by acetylation, carboxylation, and primary amine Boc-protection reactions, providing the adequate functional groups for the drug conjugation/complexation. Preliminary results on the conjugation reaction of GEM to a redox-labile linker and its characterization for later conjugation to the modified PAMAM dendrimer will be presented.



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[O-11]

Molecular identification of *Saccharomyces cerevisiae* strains from Madeira Island

Mariangie M. Castillo[1], José S. Câmara[1,2] & Mahnaz Khadem[3]

[1]*CQM - Centro de Química da Madeira, Campus Universitário da Penteada, 9020-105 Funchal, Portugal.*
[2]*Departamento de Química, Faculdade de Ciências Exatas e Engenharia, Campus Penteada, Universidade da Madeira, 9020-105 Funchal, Portugal.*
[3]*SOPlexis - Centro de Agricultura Sustentável e Tecnologia Alimentar, Campus Universitário da Penteada, 9020-105 Funchal, Portugal.*

The *S. cerevisiae* is naturally present in cerous grape skin (pruine). Its contribution to the quality and typicity of wines is well known and depends on the strain that predominates during alcoholic fermentative processes. Intraspecific diversity depends on agroedaphoclimatics conditions of the vineyards, due to selective adaptation to ecosystems [1].

In Madeira Island, the identification of *S. cerevisiae* strains is at an early stage [1]. Thus, in order to better characterization and conservation this important part of vitiviniculture heritage, the present study aims to characterize strains of *S. cerevisiae* at molecular level by analysing the interdelta polymorphism.

During 2020 campaign, 4 grape varieties from 4 certified vineyards located at north of Madeira Island, namely, *Sercial*, *Verdelho, Malvasia de São Jorge* (white grape) and *Tinta Negra* (red grape) were sampled. The grape musts were submitted to spontaneous microfermentation in controlled conditions, aseptically. A total of 120 isolates were, randomly, selected in the final phase of microfermentation [2]. All the isolates belonged to *S. cerevisiae* species [3]. Commercials strains were used as positive control. From each sampled, 1 to 4 strains were identified by the interdelta polymorphism analysis [3].

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[O-12]

A fluorinated dendrimer for traceable gene delivery

Lydia dos Orfaos, Helena Tomás & João Rodrigues*

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

Properties such as a well-defined 3D structure, internal void spaces, and the ability of functionalization of their terminal groups make dendrimers very interesting for drug/gene delivery vehicles [1]. The incorporation of Fluorine in several drugs improved their bioavailability, protein-ligand interaction, and metabolic stability [2,3]. It also has been shown to increase transfection efficiency both in vitro and in vivo in polymers [4].

This work aimed at the fluorination of generation 4 poly(amidoamine) dendrimers ($PAMAMG_4$-NH_2) with 2,3,5,6- tetrafluoro-4-hydroxybenzoic acid (TFHBA) to obtain a new magnetic resonance imaging (MRI) traceable gene delivery vector [5]. The non-fluorinated 4-hydroxybenzoic acid (HBA) was also used for comparison purpose. The functionalization of the dendrimer with the TFHBA or HBA compounds was done by dropwise addition of the compounds at different compound/dendrimer ratios, into a stirring commercial $PAMAMG_4$-NH_2 solution and left for 48h. Dialysis was performed and the obtained dendrimers with different functionalization degrees were characterized by NMR (e.g., ^{19}F, ^{1}H, ^{13}C), FTIR, UV/visible, fluorescence, and elemental analysis. pDNA condensation ability was assessed by the PicoGreen® assay and cytotoxicity was evaluated using HEK 293T cells and the resazurin metabolic activity assay. Transfection efficiency was studied using the green fluorescence protein (GFP), and the luciferase reporter genes, by fluorescence microscopy and enzyme activity determination, respectively.

The structural data confirmed the conjugation with reaction yields ranging from 88% to 97%. The biological studies revealed that the degree of functionalization impacts the cytotoxic behaviour of the conjugates. High compound/dendrimer ratios were noncytotoxic at concentrations up to 90 µg/mL, being the TFHBA conjugates less cytotoxic than $PAMAMG_4$-NH_2 and the HBA counterparts. The condensation of pDNA and transfection is shown to be better for the fluorinated dendrimers than for the $PAMAMG_4$-NH_2 dendrimer by itself.

The low cytotoxicity, good transfection efficiency, and ease of synthesis of these fluorinated dendrimers make them interesting as potential new gene delivery vectors. Antibacterial activity of the compounds and their possible use against HIV and/or cancer are work in progress.

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[O-13]

Polyphenolic profile, antioxidant and anti-diabetic potential of berries-producing plants after *in vitro* gastrointestinal digestion

Joana Pinto, Vitor Spínola & Paula C. Castilho

CQM - Centro de Química da Madeira, Campus Universitário da Penteada, 9020-105, Funchal, Portugal.

Fruits and vegetables consumption have been associated with chronic diseases prevention, including cardiovascular diseases, diabetes, cancer, and others involving inflammatory processes. Berries are rich in polyphenols, which antioxidant properties contribute to the maintenance of human health. The aim of this work was the study of the morphologic parts (berries and leaves) of berries-producing species, including *Elaeagnus umbellata*, *Rubus grandifolius*, *Sambucus lanceolata*, *Vaccinium padifolium* and *Vaccinium cylindraceum*. The impact of simulated gastrointestinal digestion on the stability of phenolic compounds and changes on their potential bioactivities was also investigated.

The analysis of the phenolic profile by HPLC-DAD-ESI/MS^n, in the negative mode, of the methanolic extracts showed that leaves have a higher content of polyphenols, compared to berries. Hydroxycinnamic acids (caffeic, coumaric and ferulic acid derivatives), caffeoylquinic acids and *O*-glycosilated flavonols (derivatives of quercetin and kaempferol) are predominant in these species.

Furthermore, the positive mode analysis allowed the identification of glycosylated anthocyanins (delphinidin, cyanidin, petunidin, peonidin and malvidin). The *in vitro* gastrointestinal digestion allowed to understand its influence on the antioxidant activity of the extracts. After digestion, leaves still showed higher antioxidant capacity than the berries. Additionally, it was found that the enzymes present in this process have less influence than the pH and ionic strength of the digestive juice. The *in vitro* inhibitory effects of the extracts on digestive enzymes responsible for the metabolism of carbohydrates, showed that the extracts were more active inhibitors of α-glucosidase than of α-amylase activity.

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[O-14]

Hyperhomocysteinemia and oxidative stress in vascular disease: Evalution of glucose-6-phospahte dehydrogenase in HUVEC cells

Isabel Faria[1,3], Mariana Vieira[1], Celso Cunha[3] & Helena Caldeira[1,2]

[1]CQM - Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal.
[2]FCV - Faculdade de Ciências da Vida, Ciclo Básico de Medicina, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal.
[3]HMT - Institute of Hygiene and Tropical Medicine, Universidade Nova de Lisboa, R. Junqueira 100, 1349-008 Lisbon, Portugal.

Hyperhomocystenemia (HHcy) is a metabolic condition characterized by the excess of homocysteine (Hcy), a sulfur-containing non-proteinogenic amino acid produced in the methionine (Met) metabolic pathway. HHcy is considered an independent risk factor for cardiovascular, cerebrovascular, cancer and other diseases. Unfortunately, it is still not clear if it has a causative effect or if it is a consequence from these diseases. *In vitro* studies have shown that an accumulation of Hcy can result in oxidative stress, which can lead to endothelial dysfunction, increased thiolation and homocysteinylation of proteins, dysruption of methylation processes used in the cellular biosynthesis of different compounds, and the methylation status of several genes [1]. One particular gene that can be affected is the Glucose 6 Phosphate Desidrogenase (*G6PD*), from which is produced the main intracellular antioxidant enzyme (G6PD), the major source of NADPH used in the antioxidant glutathione system, among others [2].

The aim of our study is to evaluate the effect of HHcy on the expression and activity levels of G6PD and their impact in oxidative stress *in vitro*. Human umbilical vein endothelial cells (HUVEC) are being used in this work. NADPH levels will be evaluated by spectrophotometric techniques, and G6PD translational and transcriptional activity by qPCR and Western-blot techniques.

This study will help to understand better if Hcy can be a valid and useful biomarker to predict the risk of development and/or of progression of various diseases.

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[O-15]

Immobilization of β-galactosidase in calcium alginate beads

Gonçalo Nuno Martins, Onofre Figueira & Paula C. Castilho

CQM - Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal.

Enzyme immobilization comprises several methodologies that take advantage of the properties of different support materials for improving enzymatic processes. Amongst many techniques, the entrapment of enzymes in calcium alginate beads is one of the simplest and most used. β-galactosidase is an enzyme relevant in the food industry for its ability to catalyze the hydrolysis of lactose into its constituent monomers, glucose and galactose, and producing lactose-free consumer goods [1].

A mixture of alginic acid and β-galactosidase at 10 U/mL was incorporated, drop-wise, into a calcium chloride solution, entrapping the enzyme in calcium alginate beads. The activity of the loaded beads was assessed by the *O*-nitrophenyl β-D-galactopyranoside (ONPG) assay, by measuring the increase in absorbance at 405 nm for 10 min at 37 °C. The immobilized system was found to have an average of 0.6 U/g bead.

To compare the hydrolysis of lactose, before and after the immobilization, reaction mixtures at 1 U/mL were prepared for both systems. In the experiments, the enzyme was incubated with lactose solutions in tris-HCl buffer pH 7.3, and the reactions were monitored for 24 h at 37 °C. Several aliquots were recovered, the enzyme was inactivated by heating at 100 °C for 10 min, and the samples were filtered, and then analyzed in the HPLC-RI. By comparing the initial and final lactose concentrations, the free enzyme was determined to having hydrolyzed 91 % of lactose, whereas the immobilized system was capable of hydrolyzing 99 % of lactose.

The comparable activity of the immobilized enzyme, against the free analogue, alongside with the possibility of recovery and reusability of the catalyst in several cycles, proves the success of this methodology. The use of green products and materials is another plus side to this strategy, allowing its use in industrial processes where β-galactosidase is present, namely for food and health-related applications.

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[O-16]

Establishment of urinary volatomic profiles for the identification of putative prostate cancer biomarkers

Cristina Berenguer[1], Ferdinando Pereira[2], Ricardo Sousa[3], Jorge A. M. Pereira[1] & José S. Câmara[1,4]

[1]CQM – Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal.
[2]SESARAM - Serviço de Saúde da Região Autónoma da Madeira, EPERAM, Hospital Dr. Nélio Mendonça, Avenida Luís de Camões 6180, 9000-177, Funchal, Portugal.
[3]Liga Portuguesa Contra o Cancro - Núcleo Regional Madeira, Rua Elias Garcia, 9050-023, Funchal, Portugal.
[4]Departamento de Química, Faculdade de Ciências Exatas e Engenharia, Universidade da Madeira; Campus da Penteada, 9020-105 Funchal, Portugal.

Prostate cancer (PCa) is the second leading cause of cancer death in men, after lung cancer. In Portugal, its occurrence has increased over the last 5 years. Family factors, age, diet, and race (higher incidence in Black race) are the most important risk factors associated with PCa. Rectal examination, transrectal ultrasound, prostate-specific antigen (PSA) blood test and prostate biopsy are the diagnostic methods commonly used. However, the lack of accuracy in the current diagnostic methods, along with the high costs and side effects, makes it urgent to develop new diagnostic tools with high sensitivity and specificity. Recently, endogenous volatile metabolites, present in different biological fluids, emerged as a promising and non-invasive approach. The aim of this work was to establish the urinary volatile profile of PCa patients (PCa group), subjects who had a prostatectomy (SP group) and healthy individuals (control (CTRL) group), to identify and define a set of molecular biomarkers for the diagnosis of PCa. Headspace solid-phase microextraction (HS-SPME) was used followed by gas chromatography-mass spectrometry (GC-MS) analysis. The data obtained were submitted to advanced statistical tools ((Principal Component Analysis (PCA)) for the selection and definition of potential molecular biomarkers. A total of 31 urinary volatile organic metabolites (uVOMs) were identified in the interventional groups, belonging to different chemical families, including ketones, terpenes, norisoprenoids, aromatic, fatty acids, alcohols, phenolic, furanic, and sulphur compounds. The chemical families with the higher contributions to the urinary metabolomic profile of the three groups were terpenes, phenolic compounds, ketones, and norisoprenoids. Between the CTRL group (n = 11), the SP group (n = 13) and the individuals with PCa (n = 11), the urinary levels of 12 of the 31 uVOMs were found to be statistically significant ($p < 0.05$, ANOVA test). The PCA analysis showed two defined clusters corresponding to the CTRL and PCa groups. Some individuals in the SP group seem closely related to the CTRL group, while others have a volatomic profile similar to the cancer group. The results showed the potential of the methodology used in the discovery of urinary biomarkers, uVOMs, for the diagnosis of PCa. Robustness of the results will be achieved with the analysis of a higher number of samples.

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[O-17]

Induction of the osteogenic differentiation of human Mesenchymal Stem Cells by Protamine/pDNA/PAMAM-COOH ternary complexes

Fátima Moreira[1,2], Filipe Olim[1], Helena Tomás[1*] & Rita Castro[1**]

[1]*CQM – Centro de Química da Madeira, Universidade da Madeira, Campus da Penteada, 9020-105 Funchal, Portugal. *lenat@staff.uma.pt, **ritacastro@staff.uma.pt*
[2]*Departamento de Ciências da Vida, Faculdade de Ciências e Tecnologia, Universidade NOVA de Lisboa, Campus da Caparica, 2829-516 Caparica, Portugal.*

Mesenchymal Stem Cells (MSCs) are non-haematopoietic and multipotent cells with the capacity to differentiate into different cell types, including osteoblasts, chondroblasts and adipocytes [1,2]. The delivery of osteogenic genes using nanomaterials, scaffolds or other delivery systems can induce the direct differentiation of MSCs into osteoblastic cells. Thus, gene therapy is a promising tool to promote bone formation and regeneration in pathological settings [3,4]. Additionally, Bone Morphogenetic Protein (BMP)-2, an osteogenic differentiation factor, has been reported to induce the *in vitro* differentiation of MSCs towards the osteoblastic lineage [5].

In this work we propose a novel non-viral hybrid transfection system composed of protamine sulfate (PS), plasmid DNA (pDNA) and carboxylate-terminated poly(amidoamine) dendrimer (PAMAM-COOH) to induce the osteogenic differentiation of human MSCs (hMSCs). This ternary complex was firstly prepared by the condensation of pDNA with PS forming a positive-charged binary complex, and then further interaction with the anionic dendrimer.

The physical and chemical properties of the binary and ternary complexes, as well as their biological performance were assessed. The binary PS/pDNA complexes successfully condensed and neutralized pDNA charge, and protected pDNA from serum nucleases digestion, despite exhibiting a low transfection efficiency *in vitro* (the GFP and luciferase reporter genes were used in these studies). Following, the addition of PAMAM-COOH, that effectively interacted with PS/pDNA forming a ternary complex, revealed an enhanced transfection efficiency, being dendrimer generation and dendrimer/pDNA ratio-dependent. In addition, ternary PS/pDNA/PAMAM-COOH complexes with pDNA encoding for human BMP-2 and generation 4.5 PAMAM-COOH were used to induce the osteogenic differentiation of hMSC, which was evaluated qualitative and quantitatively. Preliminary results indicate that the proposed hybrid transfection system induced an initial differentiation of hMSCs towards the osteoblastic lineage.

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Participants List

Participant
Ana Carolina Coelho Rodrigues
Ana Filipa Gonçalves Rodrigues
Beatriz Gomes Jardim
Carolina Fátima Pereira Andrade
Cristina Viveiros Berenguer
Dina Maria Sousa Maciel
Fátima José Batista Moreira
Fátima José Mendes Ferreira
Filipa Nunes Pita
Filipa Raquel Nunes Jardim
Gonçalo Nuno Gouveia Martins
Helena Cristina Silva Chá-Chá
Helena Maria Pires Gaspar Tomás
Isabel Pereira Faria
Ivo José Viveiros Martins
Jaison Jeevanandam
Joana Carolina Nunes Pinto
João Manuel Cunha Rodrigues
Joaquim Duarte Gonçalves Fernandes
Jorge A. M. Pereira
José Carlos Almeida Mesquita
José João Caires Serina
José S. Câmara
Letícia Míriam de Sousa Joaquim

Participant
Lydia Nadège Abreu dos Orfaos
Mara Isabel Jesus Gonçalves
Mariana Catanho da Silva Vieira Soares
Mariangie Elisa Martinez Castillo
Nádia Sofia Henriques Nunes
Onofre Agapito da Silva Figueira
Paula Cristina Machado Ferreira Castilho
Patrícia Maria Gonçalves Sousa
Pedro Filipe Duarte Louzeiro Pires
Rita Maria de Castro
Rosa Perestrelo
Rui Miguel Vieira Ferreira
Ruilong Sheng
Vanessa Silva Santos

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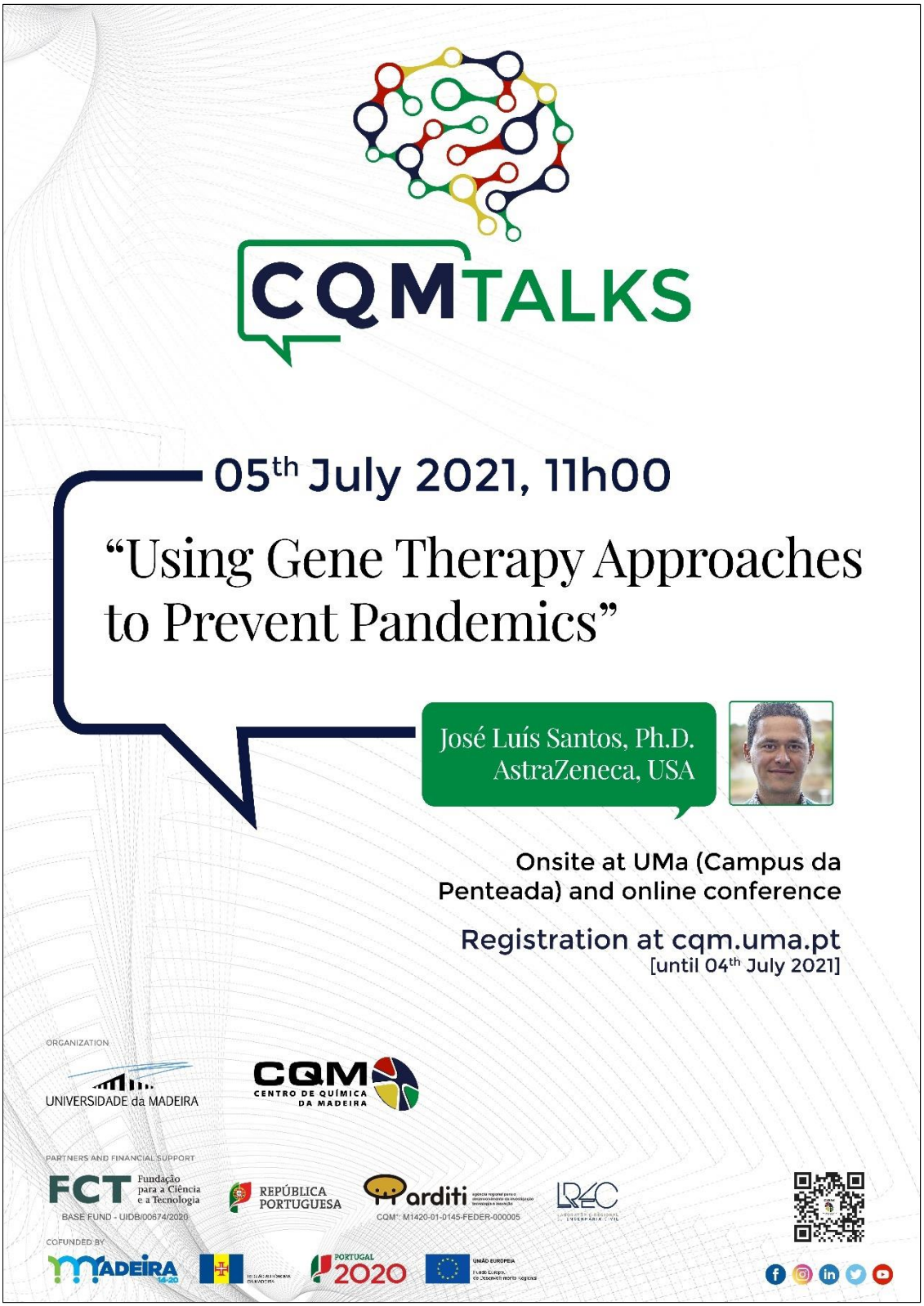

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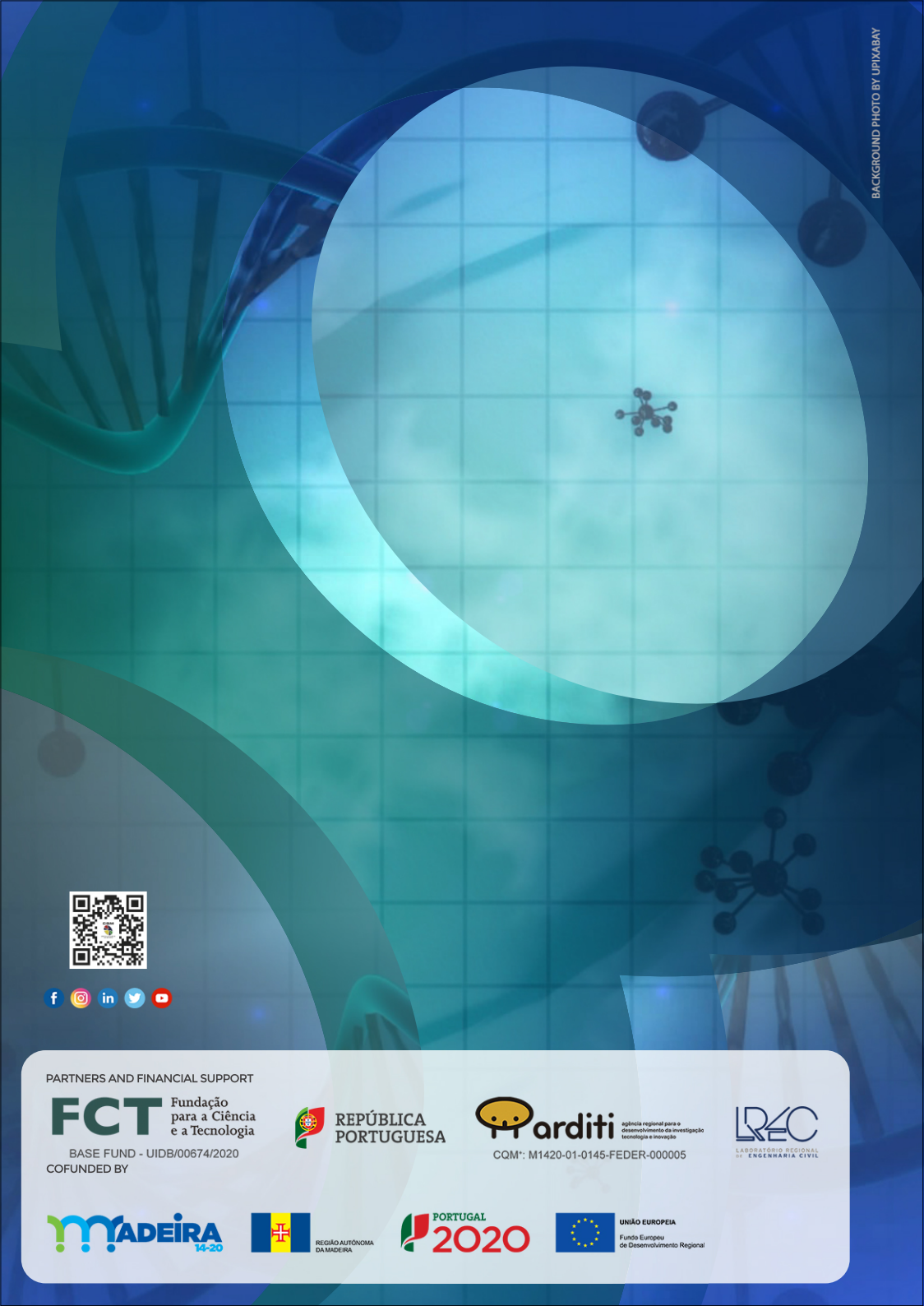

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