CQM
CENTRO DE QUÍMICA
DA MADEIRA

UNIVERSIDADE da MADEIRA

7TH CQM ANNUAL MEETING

ABSTRACT BOOK

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2020

21-22 September

AUDITÓRIO DO COLÉGIO DOS JESUÍTAS

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7TH CQM ANNUAL MEETING

CQM CENTRO DE QUÍMICA DA MADEIRA

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About CQM

Governance Structure

Executive Committee (2019-2020)

João Rodrigues	*Scientific Coordinator*
Helena Tomás	*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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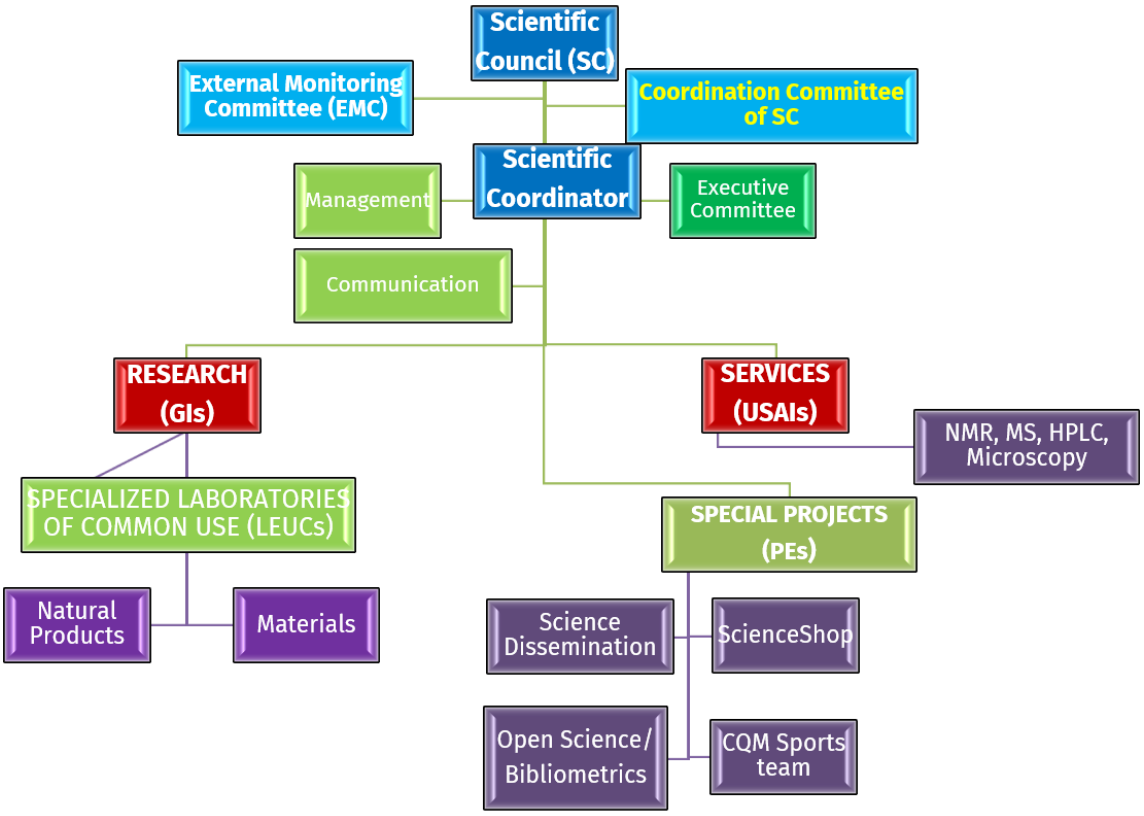
José Martinho Simões	*Full Professor FCUL - Faculdade de Ciências, Universidade de Lisboa, Portugal*
Abhay Pandit	*CÚRAM, Centre for Research in Medical Devices, National University of Irland*
Makoto Fujita	*Full Professor, Department of Applied Chemistry, University of Tokyo, Japan*
John Beutler	*National 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.

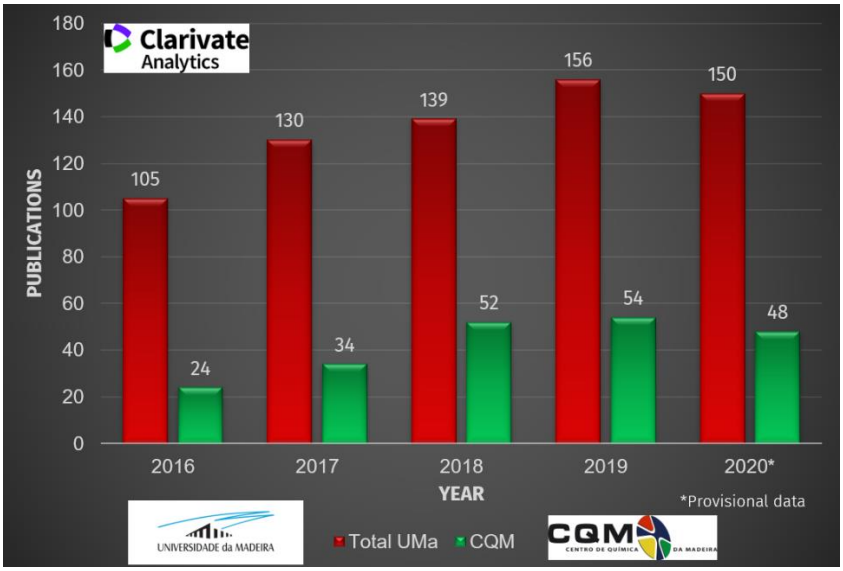
CQM Commitments and Principles

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 – A door opens to the future

When a handful of Ph.D. researchers from the Department of Chemistry decided, in 2004, to create a research centre in Chemistry at the University of Madeira, it was not only guaranteeing the future of the area in the Region but also unequivocally contributing to the future of the university itself. Effectively, the impact of the existence of CQM is not only measured by its scientific production, by the dissemination of science and by services to the community, but also by the scientific support given to the courses, especially those led by the Department of Chemistry. Together with a vision of internationalization of knowledge and of responding to the needs of the Region in the most emblematic industrial sectors, the commitment made by CQM in the training of human resources was decisive to ensure not only its future but also the future of the courses it supports. Naturally, without the existence of CQM, the 1st Cycle in Biochemistry, the Master in Applied Biochemistry, the Master in Nanochemistry and Nanomaterials, and particularly, the Ph.D. in Chemistry, would hardly be accredited by the Higher Education Evaluation and Accreditation Agency (A3ES). Besides, without human resources trained locally, not only would we not have been able to materialize the international affirmation of CQM and UMa, but it would not have been possible to respond to the needs of the Region in highly qualified human resources.

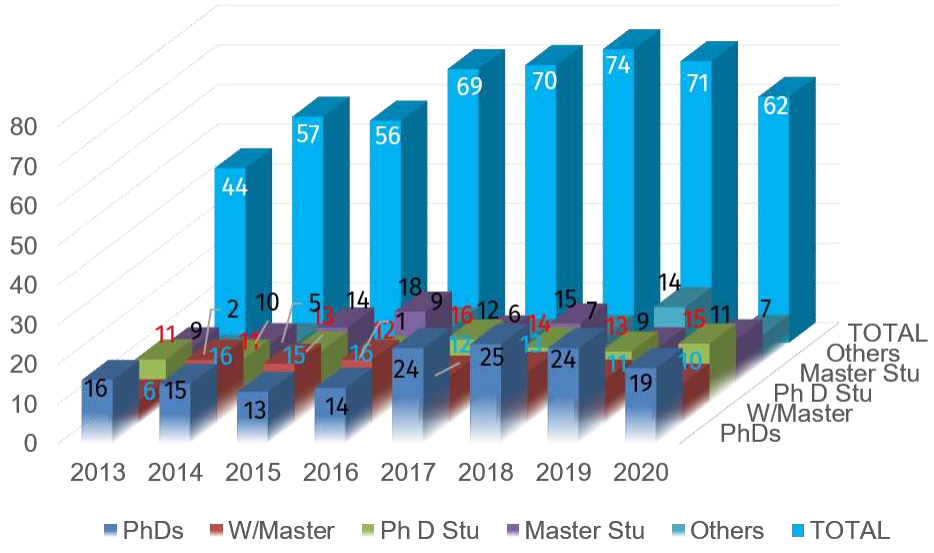


- CQM Publications 2016-2020.

In this path that led us to publish, in 2019, 54 articles (with an average impact factor of 4.5) and to be recognized nationally and internationally, CQM has developed, in its short past, a set of activities far beyond what would be expected given its size, available resources, and geographical location. Others, with superior resources and dimensions, with centralities that allowed them to influence fundamental decisions, took much

longer to assert themselves or disappeared along the way. Indeed, the impact of CQM's work in terms of knowledge production at the University of Madeira and the Autonomous Region of Madeira has been highlighted, not only by the successive international evaluation panels of FCT but also in several national and international reports. As reported on a publication from Francisco Manuel dos Santos Foundation published in 2019 ("The evolution of science in Portugal (1987-2016)"), CQM appears prominently in the geographical space of Madeira and the Azores, not only for its contribution to the specialization of knowledge in the University of Madeira in the areas of Chemistry and Medical Engineering and Nanotechnology but also in the area of Industrial Biotechnology, which led the authors to write "In the case of UMa, the index of specialization is very high for Industrial Biotechnology, publications that are, for the most part, the responsibility of the Madeira Chemistry Research Centre".

In the successive FCT assessments and given the work developed, it has always been recognized the audacity of CQM to want, in a young university, of small dimension and in the middle of the Atlantic, to be equal, or even better, than other centres in the country. However, the evaluators never dared to assume that a small and geographically peripheral research unit should be financed in the exact proportion of its merit.



- CQM research team evolution (2013-2020).

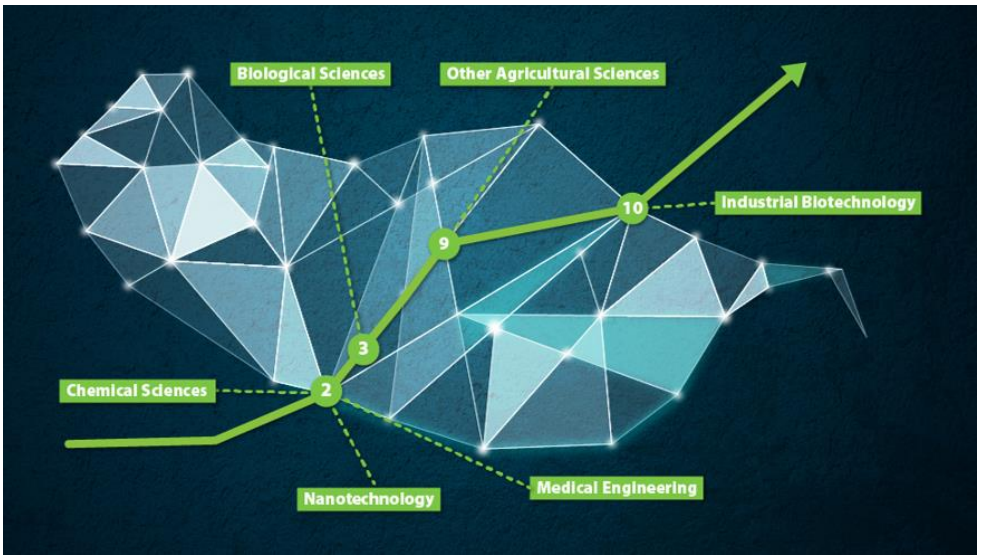
In fact, so that a unit of our size can continue to develop and serve the Region and the Country, it is necessary to ensure regular funding that allows not only to recruit the best in the global market but also to keep our best Ph.D. students. This recruitment capacity is not only dependent on the available funding, which varies according to the evaluation cycles and European funding programs, but, more than ever, limited by the legislation, fair in principle, but blind in its application to the national whole. This situation prevents us, for example, to hire young Ph.D. graduates from CQM as scholarship holders.

Another aspect is related to the need for regular auditable funding that allows the maintenance of a minimum infrastructure that supports the 4 main pillars of CQM activity (research/training/dissemination/services), helping to change the operating paradox of the CQM itself. Its current operation model relies too much on doctoral and postdoctoral students who take on tasks that should be performed by a minimum permanent body of research technicians and administrative staff with higher education, thus leaving researchers more available time for scientific work. The CQM ability to provide services is, of course, supported by these researchers who, when asked to do so, have to interrupt their research projects to respond to a need for service provision submitted by a public or private entity. And at what cost?

The existence of a small technical/administrative and communication framework was, in part, achieved with the CQM^{+} operation (financed under Madeira 14-20, Operational Program of the Autonomous Region of Madeira). The conclusion of this operation in the short term will, however, dismantle this minimal support structure, with the aggravation of, once again, seeing many of our highly qualified trainees leave for other places or find themselves forced to change careers.

To remain competitive at the national and international level, and contribute to the national and regional strategy of smart specialization, CQM has to:

a) Find regular funding that allows it to maintain a stable body of 20-25 PhDs;
b) Have a permanent technical/administrative body;
c) Together with the University, Regional and National Government, find a way to comply with the "Programa de Regularização Extraordinária dos Vínculos Precários na Administração Pública (PREVPAP. Lei n.° 112/2017, de 29 de dezembro)" and to respond to the legitimate aspirations of those who, practically without rights, have given their best effort for the improvement of research, technological development, and innovation in the Region and Country;
d) Not only to invest in the renovation of spaces and equipment but also to pursue the ongoing policy of bringing to the region equipment that does not exist here, that can be shared, and that enhance our ability to compete internationally;
e) Continue to have the capacity to attract highly qualified human resources in the international market to complement the existing critical mass and with the potential to bring more scientific and financial value to CQM and to the Region;
f) Reinforce their integration in national and international research consortia.



- CQM scientific areas contribution.

By 2023, CQM has a commitment to fulfil, which is to execute the strategic plan approved by FCT. Most likely, in 2022 or 2023, we will start a new evaluation cycle. What happens in the next 2 years will be decisive for the success of the evaluation of the Centre. However, if a substantial part of the work required for success assessment is in our hands, another part is dependent on the ability to carry out what has been said above, the existence of a stable body of researchers and technicians. As seen in previous evaluations, the quality and quantity of publications alone, being important, are not sufficient to reach the level of funding that allows us to go further.

Thinking today on what we should become 10 years from now, despite the uncertainties, is not a chimera, but an opportunity to project for the future. Without doing that in the past, we would not be here today, available to give our contribution whenever the circumstances so require.

Something that the pandemic has shown us is the importance of knowledge and the need to have the capacity to produce it. During the confinement, we were at the service of the Region in what the authorities considered we were useful for. The creation of the Laboratory of the Future (Operation CQM^{+}) would allow us, if it had been necessary, to go even further in participating in this joint effort to fight the COVID-19 disease that is affecting populations worldwide.

The projects that CQM has in its portfolio, that is, those already submitted to FCT and the Regional Government under the Regional Investment Plan 2030 are not mere financial allocation exercises. They are the manifestation of an imperative of conscience that tells us that for a Country/Region to assert itself economically and create jobs, it must train very well the people and invest in fundamental/applied knowledge and innovation.

In conclusion, considering the thematic areas of smart specialization, Health, Agrofood, Biodiversity, Sea, the document under public discussion "Strategic vision for the economic and social recovery plan of Portugal 2020-2030", and also the "Manifesto of the 100", CQM considers that the economy of the country and the Region require a long-term investment of national/regional basis in high-quality human resources, in ecosystems and technological infrastructures for fundamental/translational science and cutting-edge innovation, in the universities, research units and companies, complementary to the European Funds. This investment is even more important for the peripheric of the Regions. The work carried out by CQM and its impact on the Region is proof that investments in research units, even small and without an economy of scale, but with highly motivated, organized teams with international experience and recognition, can create jobs, boost the production of knowledge with economic impact, give international visibility to the Region and the Country, and even respond to emergencies like the one we are currently living in.

At a time of so many uncertainties, it is now important to fulfil this greater purpose, which is to realize hope. From the CQM side, we will be here, ready to take advantage of the opportunities given to us so that the impact of knowledge is a reality in the Regional economy and the well-being of the society.

University of Madeira, Funchal, 21st September 2020

(João Rodrigues, Scientific Coordinator of CQM)

Program

Monday, 21st September 2020

10:00	10:45	**Opening session** **Professor José Carmo** *Rector of the University of Madeira* **Dr. Jorge Carvalho** *Regional Secretary for Education, Science and Technology* **Professor João Rodrigues** *Scientific Coordinator of CQM*
10:45	11:15	**Coffee-break**
Chairperson: Jorge Pereira		
11:15	11:45	[O-01] **pH/redox Dual stimuli-responsive nanomaterials for controllable drug release** Ruilong Sheng
11:45	12:05	[O-02] **Fish quality evaluation from Madeira aquaculture production. Freshness analysis and rejection day estimation, through complementary approaches** Jorge Freitas, Paulo Vaz-Pires & José S. Câmara
12:05	12:25	[O-03] **Biological activity of ruthenium metallodendrimers: *in vitro* and *in vivo* studies** Dina Maciel, Yu Fan, Gaoming Li, Xiangyang Shi, Helena Tomás & João Rodrigues
12:25	12:40	[O-04] **An analytical tool for inulin hydrolysis - can I use my smartphone in the lab?** Onofre Figueira & Paula C. Castilho
12:40	12:55	**Group photo**
12:55	14:30	**Lunch**
14:30	14:55	**Signature of terms of office for new CQM members**

Chairperson: Mara Gonçalves		
14:55	15:20	[O-05] **PAMAM dendrimer as delivery system for the stimuli-responsive release of gemcitabine and *cisplatin* for the treatment of pancreatic cancer** Rita Castro, Helena Tomás & João Rodrigues
15:20	15:35	[O-06] **Correlation of chromatographic and spectrometric methodology for characterization and profiling of marine oils – "how about polar lipids?"** Rui Ferreira, Marijana Petković & Paula C. Castilho
15:35	15:55	[O-07] **Nanoplatforms based on self-assembly of cholesterol-doxorubicin conjugated lipid with TPGS** Filipe Olim, Ana Rute Neves, Mariana Vieira, Helena Tomás & Ruilong Sheng
15:55	16:15	[O-08] **Chemical characterization of twelve seized products suspected to contain synthetic cathinones** João Gonçalves, Vera Alves, Joselin Aguiar, Maria J. Caldeira, Helena M. Teixeira & José S. Câmara
16:15	16:35	[O-09] **Piezoelectric PVDF/MWCNTs electrospun nanofibers as a platform for biological applications** Huang Wei, Xiangyang Shi & Pedro Pires
16:35	17:05	**Coffee-break**
Chairperson: Mariana Vieira		
17:05	17:20	[O-10] **Laponite®-based nanogels for bone tissue regeneration and treatment of osteoporosis** Fátima Mendes, Filipe Olim, Ana Rute Neves, Mariana Vieira, João Rodrigues & Helena Tomás
17:20	17:35	[O-11] **The fluorination of poly(amidoamine) (PAMAMG4-NH2) dendrimers - synthesis characterization and biological studies** Lydia dos Orfaos, Helena Tomás & João Rodrigues
17:35	17:55	[O-12] **From fish transforming industry residues to biomaterials: a characterization of hydroxyapatite-based materials extracted from fish by-products** Pedro Ideia, Lorenzo Degli Esposti, Carla Caseiro Miguel, Alessio Adamiano, Michele Iafisco & Paula C. Castilho
17:55	19:25	**General meeting with CQM members**

Tuesday, 22nd September 2020

Chairperson: Rita Castro		
09:00	09:25	[O-13] **Platinum IV complexes conjugated with bis-MPA dendronised PEG: synthesis and characterization** Mara Gonçalves, Helena Tomás & João Rodrigues
09:25	09:40	[O-14] **Rapid screening and analytical characterization of synthetic cannabinoids in 'herbal incenses'** Vera Alves, João Gonçalves, Joselin Aguiar, Maria J. Caldeira, Helena M. Teixeira & José S. Câmara
09:40	10:00	[O-15] **PAMAM dendrimers – a strategy to improve the efficacy of 1,2-diaminocyclohexane platinum(II)** Cláudia S. Camacho, Helena Tomás & João Rodrigues
10:00	10:15	[O-16] **Exploring the controlled growth of copper-based nanoparticles** Duarte Fernandes, Carla S. Alves, João Rodrigues & Pedro Pires
10:15	10:30	[O-17] **Electroactive polymer-metal composite fibres** Carla Caseiro Miguel, Duarte Fernandes, Pedro Pires & João Rodrigues
10:30	11:00	**Coffee-break**
Chairperson: Jorge Pereira		
11:00	11:20	[O-18] **Metabolic profile of cells in the presence of cinnamic acid-terminated dendrimers** Ana Olival, Helena Tomás & João Rodrigues
11:20	11:35	[O-19] **Novel dendrimer-based nanoparticles for targeted computed tomography imaging of cancer cells** Nilsa Abreu, Carla S. Alves, Helena Tomás, Xiangyang Shi & João Rodrigues
11:35	11:50	[O-20] **Surface modification of carbon dots with 4-aminobenzonitrile through amide coupling reaction** Ivo J. Martins, Rita Castro, Helena Tomás & João Rodrigues
11:50	12:05	[O-21] **Development of bacteriophage-based bionanosensors for the diagnosis of infectious diseases using the phage display technique** Helena Chá-Chá, Mariana Vieira, João Rodrigues, Helena Caldeira & Helena Tomás

12:05	12:20	[O-22] **Unveiling the mechanism of action of novel anticancer candidates – [Ru(η5-C5H5)(PPh3)2]-PAMAM metallodendrimers** Nádia Nunes, Helena Tomás & João Rodrigues
12:20	12:50	**Closing session**

Oral Communications

[O-01]

pH/redox Dual stimuli-responsive nanomaterials for controllable drug release

Ruilong Sheng

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Developing smart nano-drug delivery systems (DDSs) has attracted great attention in the past decades [1]. Many mono-stimuli (pH, bioreduction/redox, light, magenetic field, enzymes) responsive nano-DDSs have been developed [2], they demonstrated better delivery capability than morphology-controlled and hydrophobicity-controlled drug release systems [3]. Nevertheless, microenvironments of tumor cells/tissues generally have both acidic (low-pH) and bioreduction/redox (Cys/GSH) features. Thus, design pH/redox dual stimuli-responsive nanomaterials with good biocompatibility and high delivery efficiency towards time/spatial- controlled drug release, is a challenging area and need to be greatly investigated.

In this work, a series of PDPA-b-P(NMS-co-OEG) diblock terpolymers (P1–P3) were prepared via reversible addition-fragmentation chain transfer (RAFT) polymerization and were characterized, which were self-assembled in solution to form noncross-linked (NCL) nanomicelle (sizes: 30–90 nm), then the NCL micelles were *in situ* crosslinked with redox-responsive cystamine to prepare shell-cross-linked (SCL) micelles. Using the optimized PDPA33-b-P(NMS22-co-OEG25) P3-micelles as the model, the pH/redox-dual responsive properties were studied by DLS and NMR. For drug delivery application, the antitumor drug camptothecin (CPT)-loaded P3-NCL and P3-SCL micelles were prepared and the related drug loading efficiency, pH/redox-dual responsive behaviors were studied by fluorescence spectrometer [4].

References: [1] Liu, D.; Yang, F.; Xiong, F.; Gu, N. *Theranostics* **2016**, *6*: 1306. [2] (a) Karimi, M.; Ghasemi, A.; Zangabad, P.; Rahighi, R.; Basri, S.; Mirshekari, H.; et al. *Chem. Soc. Rev.* **2016**, *45*: 1457.; (b) Cheng, R.; Meng, F.; Deng, C.; Klok, H.; Zhong, Z. *Biomaterials* **2013**, *34*: 3647. [3] (a) Wang, Z.; Luo, T.; Cao, A.; Sun, J.; Jia, L.; Sheng, R. *Nanomaterials* **2018**, *8*: 136; (b) Wang, Z.; Luo, T.; Sheng, R.; Li, H.; Sun, J.; Cao, A. *Biomacromolecules* **2016**, *17*: 98. [4] Sun, J.; Wang, Z.; Cao, A.; Sheng, R. *Rsc Advances* **2019**, *9*: 34535.

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[O-02]

Fish quality evaluation from Madeira aquaculture production. Freshness analysis and rejection day estimation, through complementary approaches

Jorge Freitas[1], Paulo Vaz-Pires[2,3] & José S. Câmara[1,4]

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[3]CIIMAR – Centro Interdisciplinar de Investigação Marinha e Ambiental, Terminal de Cruzeiros de Leixões, Av. General Norton De Matos, S/N, 4450-208 Matosinhos, Portugal
[4]Faculdade de Ciências Exatas e Engenharia, Universidade da Madeira, Campus Da Penteada, 9000-390 Funchal, Portugal

In the food industry, quality is frequently defined using terms related to nutrition, microbiology, physicochemical characteristics or consumer acceptability. These terms should be analysed through an integrated vision since all of them contribute to quality assessment in different steps of the supply chain. Freshness is one of the basic contributors to quality and safety of seafood products, that can be assessed through similar approach as quality, but associated with the progression of fish spoilage, also allowing to estimate its capability to retain optimal characteristics until the time it is processed, cooked, presented or eaten [1].

In this work, freshness of two fish species produced in aquaculture in Madeira (*Seriola dumerili* and *Sparus aurata*) were evaluated using, sensory analysis through Quality Index Method, chemical analysis through TMA quantification with HS-SPME/GC-MS, physical analysis with Torrymeter, and microbial analysis through colonies counts, in order to estimate its shelf-life.

For *Sparus aurata*, the estimated rejection day was 9 days, from chemical analysis was 8-9days when while for sensory was 7-8days, physical 8-9 days and microbial analysis 9-10days. In the case of *Seriola dumerili* the rejection was estimates as 12 days with the following results for each analysis, chemical 12-13 days, microbial 10-11 days, physical 11-12 and sensory 11-12 days [2].

This work results will contribute to the improvement of the knowledge and quality of the developing aquaculture sector in Madeira.

References: [1] Freitas, J.; Vaz-Pires, P.; Câmara, J.S. *Aquaculture*. **2020**, 518: 734857. [2] Freitas, J.; Vaz-Pires, P.; Câmara, J.S. *Molecules* **2019**, 24: 3530.

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[O-03]

Biological activity of ruthenium metallodendrimers: *in vitro* and *in vivo* studies

Dina Maciel[1], Yu Fan[2], Gaoming Li[2], Xiangyang Shi[1,2], Helena Tomás[1] & João Rodrigues[1*]

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Metal complexes have been considered as potential new anticancer therapeutics. Ruthenium complexes present less toxicity, tumour selectivity, and different oxidation states, which makes them an interesting alternative to platinum compounds [1,2].

Based on our previous work [3] we have prepared a low generation of poly(alkylidenamine)-based metallodendrimers (generation 0, 1, and 2) functionalized with the ruthenium moiety $[Ru(\eta^5\text{-}C_5H_5)(PPh_3)_2]^+$. These ruthenium metallodendrimers were characterized, and their biological activity was assessed. Also, their stability was performed by ^{1}H- and ^{31}P-NMR at three different temperatures (4, 25, and 37°C). The *in vitro* anticancer activity was evaluated against several cancer cell lines. Other biological assays were performed, such as DNA binding assays and hemolytic activity. The reactive oxygen species (ROS), the apoptosis, the mitochondrial membrane potential, and cell cycle were, as well, assessed by flow cytometry. *In vivo* studies were conducted with these metallodendrimers to examine their therapeutic efficacy (Figure 1). The cytotoxicity suggests a generation effect with increasing toxicity in higher generations. The metallodendrimers revealed a strong interaction with DNA, and induced necrosis and late apoptosis. As such, these metallodendrimers present an attractive potential to be used as anticancer metallodrugs.

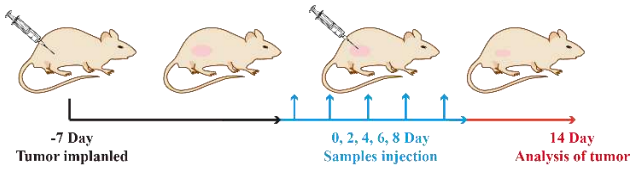

Figure 1. Representation of the *in vivo* antitumor therapy used to test the ruthenium metallodendrimers.

References: [1] Liu, J.; Lai, H.; Xiong, Z.; Chen, B.; Chen, T. *Chem. Commun.* **2019**, *55*: 9904. [2] Thangavel, P.; Viswanath, B.; Kim, S. *Int. J. Nanomed.* **2017**, *12*: 2749. [3] a) Jardim, M.G.; Rissanen, K.; Rodrigues, J. *Eur. J. Inorg. Chem.* **2010**, *11*: 1729; b) Gouveia, M.; Figueira, J.; Jardim, M.G.; Castro, R.; Tomás, H.; Rissanen, K.; Rodrigues, J. *Molecules* **2018**, *23*: 1471

Acknowledgments: This research was supported by FCT-Fundação para a Ciência e a Tecnologia through the CQM Strategic Project PEst-OE/QUI/UI0674/2019, CQM Base Fund - UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020, and by the Ph.D. Grant SFRH/BD/102123/2014 (DM). The authors also acknowledge ARDITI-Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação, respectively through the project M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM$^+$ (Madeira 14-20).

[O-04]

An analytical tool for inulin hydrolysis - can I use my smartphone in the lab?

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The aim of the present work was to perform a 24 hour enzymatic hydrolysis of inulin of a yacon extract into FOS, with TLC analysis as an attempt to quantify the produced FOS before injection into HPLC.

The hydrolysis occurred in a recirculatory system with immobilized endo-inulinase for 24h, at 55 °C. The yacon extract was previously lyophilized and dissolved in sodium acetate buffer 0,1M pH 5. The reaction was analyzed by TLC at the first 4 hours and last 5 hours of the reaction. TLC was developed using the eluent butanol: acetic acid: water (2:1:1) and the spots developed with N-(1-naphthyl)ethylenediamine by heating the plate at 100 °C. The TLC method was developed to the highest spot definition possible. For the attempt of quantification by TLC, a simple picture of the developed TLC was taken with the smartphone. The image was then processed and analyzed using ImageJ software, in order to achieve an approximate quantification by densitometry. Besides the spots being easy observable in the TLC plate, the software allows the plotting of the spots into peaks in a graphic very similar to a chromatogram. The concentration values for each spot was calculated through a calibration curve done with fructose at different concentrations (0.5 to 50 g/L). In spite of having concentration values largely different from those obtained from HPLC, the ratios FOS/monosaccharides were very similar.

Despite the method lacking optimization and not being reliable for a real quantification of FOS, the TLC present a good separation between each saccharide, allowing the identification of FOS with different DP's and the obtention of ratio of saccharides with reliable values.

Acknowledgments: This work was supported by FCT (Project PEst-OE/QUI/UI0674/2019, CQM, Portuguese Government funds), and through Madeira 14-20 Program, project PROEQUIPRAM - Reforço do Investimento em Equipamentos e Infraestruturas Científicas na RAM (M1420-01-0145-FEDER-000008), ARDITI, through the project M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM+ (Madeira 14-20 Program) and by PREMIUM Horizon 2020 – MSCA – RIS E – 2017, N° 777657.

[O-05]

PAMAM dendrimer as delivery system for the stimuli-responsive release of gemcitabine and *cisplatin* for the treatment of pancreatic cancer

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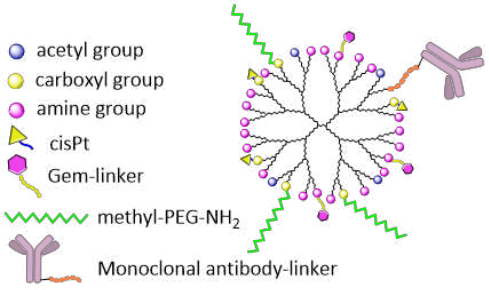
Pancreatic ductal adenocarcinoma (PDAC) is the most common pancreatic cancer type (90%), with high mortality and low 5-year survival rate (2-9%) [1]. Its treatment usually requires high doses of multiple drugs to overcome drug resistance, such as the combination of gemcitabine (Gem) and *cisplatin* (*cis*Pt), which have shown improved results, with fewer side effects and higher synergistic activity [2]. The use of a drug delivery system (DDS) like poly(amidoamine) (PAMAM) dendrimers could improve its efficacy, specificity and lower doses, leading to fewer side effects [3]. Indeed, Gem and *cis*Pt have been delivered, separately or in combination with other drugs, by PAMAM dendrimers, but never both were co-delivered (neither by dendrimers nor by other DDS) [4]. Thus, the strategy under study involves the surface modification of PAMAM dendrimer and conjugation of Gem and *cis*Pt to the PAMAM via redox and pH labile-linkers, respectively, for a stimuli-responsive and controlled drug release. The preliminary results on the PAMAM dendrimer surface modification showed, by ^{1}H NMR, the successful introduction of 21 acetyl groups (19% acetylation, 94.4 % yield), to decrease the positive surface charge, 20 carboxyl groups (18% carboxylation, 93.9% yield) for *cis*Pt conjugation and 41 boc-primary amine protecting groups (37% for protection, 61.8% yield) to avoid side reaction and unspecific interactions during Gem conjugation. Later on, for PDAC cell targeted delivery, an overexpressed cell-surface glycoprotein monoclonal antibody will be conjugated, along PEG chains for stealth effect purposes.



References: [1] Adamska, A.; Domenichini, A.; Falasca, M. *Int. J. Mol. Sci.* **2017**, *18*: E1338. [2] Ouyang, G.; Liu, Z.; Huang, S.; Li, Q.; Xiong, L.; Miao, X.; Wen, Y. *World J. Surg. Oncol.* **2016**, *14*: 1. [3] Ho, B.N.; Pfeffer, C.M.; Singh, A.T.K. *Anticancer Res.* **2017** *37*: 5975. [4] (a) Çalış, S.; Gürbüz, M.U.; Esendağlı, G.; Tülü, M.; Öztürk, K. *Int. J. Pharm.* **2016**, *517*: 157. (b) Kesavan, A.; Ilaiyaraja, P.; Beaula, W.S.; Kumari, V.V.; Lal, J.S.; Arunkumar, C.; Anjana, G.; Srinivas, S.; Ramesh, A.; Rayala, S.K.; Ponraju, D.; Venkatraman, G. *Eur. J. Pharm. Biopharm.* **2015**, *96*: 255. (c) Lin, L.; Fan, Y.; Gao, F.; Jin, L.; Li, D.; Sun, W.; Li, F.; Qin, P.; Shi, Q.; Shi, X.; Du, L. *Theranostics* **2018**, *8*: 1923.

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 projects M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM$^+$ and M1420-09-5369-FSE-000002 (Post-Doc Grant to RC) are also acknowledged for the support provided.

[O-06]

Correlation of chromatographic and spectrometric methodology for characterization and profiling of marine oils – "how about polar lipids?"

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In lipidomic, the standard approach of gas chromatography for analysis of fatty acid methyl esters (FAMEs) has been the method of choice for characterization of food oils. Fatty acid quantification requires a derivatization step to perform the esterification of FA to a volatile derivative FAME. Due to the chemical reaction and matrix polarity, this methodology may not be representative of all lipid classes presented in oils.

In this study, marine oils extracted with organic solvents were subjected to TLC with silica gel for lipid class separation, before GC-FID quantification of FA. FTIR-ATR spectroscopy, high-resolution ^{1}H, ^{13}C and ^{31}P NMR spectroscopy and MALDI-TOF-MS was also used for characterization of extracts.

The spectroscopic methodology applied provides a fast and easy insight in the molecular structure of lipid oils and relative qualification of ω-3 FA and MUFA:PUFA ratio, using very small amounts of sample and little sample preparation. These data are in direct correlation with FA profiles characterized by GC-FID. Furthermore, MALDI-TOF-MS spectrometry and ^{31}P NMR offers additional information about the co-extracted phospholipids, which the other techniques cannot provide.

Acknowledgments: This work was supported by Fundação para a Ciência e a Tecnologia (Project PEst-OE/QUI/UI0674/2019, CQM, Portuguese Government funds), and through Madeira 14-20 Program, project PROEQUIPRAM - Reforço do Investimento em Equipamentos e Infraestruturas Científicas na RAM (M1420-01-0145-FEDER-000008) 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).

[O-07]

Nanoplatforms based on self-assembly of Cholesterol-Doxorubicin Conjugated Lipid with TPGS

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Developing new functional drug delivery nanosystems with the merit of easy-to-prepare, good storage stability, low hemotoxicity, as well as controllable drug delivery, has attracted much attention in recent years [1]. In this work, we present a prodrug-based nanosystem by self-assembling of cholesterol-doxorubicin prodrug conjugate (**Chol-Dox)** and Tocopherol Polyethylene Glycol Succinate (**TPGS**) using the thin-film hydration method [2].

The **Chol-Dox**/**TPGS** assemblies (molar ratio 2:1, 1:1 and 1:2) were able to form nanoscale particles with average hydrodynamic diameter in the range 100~200 nm, and surface zeta potential of -20.6~-24.0 mv. The **Chol-Dox**/**TPGS** assemblies showed low hemotoxicity and different cytotoxicity in breast cancer cells (MCF-7 and MDA-MB-231) which largely depended on the molar ratio of **Chol-Dox** and **TPGS.** Moreover, the **Chol-Dox**/**TPGS** assemblies tend to enter into MCF-7 and MDA-MB-231 cells through non-Clathrin-mediated multiple endocytosis pathways and lysosome-dependent pathway. Additionally, the results demonstrated that the **Chol-Dox**/**TPGS** nanoassemblies could be employed as promising candidates for prodrug-based nanomaterials for combinatorial tumour chemotherapy.

References: [1] Irby, D.; Du, C.; Li, F. *Mol. Pharm.* **2017**, *14*: 1325. [2] Sheng, R.; Zhuang, X.; Wang, Z.; Cao, A.; Lin, K.; Zhu, J. *Nanomaterials* **2016**, *6*: 69.

Acknowledgments: ARDITI - *Agência Regional para o Desenvolvimento da Investigação Tecnologia e Inovação* (project M1420-01-0145-FEDER-000005-Centro de Química da Madeira-CQM+), FCT - *Fundação para a Ciência e a Tecnologia* (CQM Base Fund - UIDB/00674/2020 and Programmatic Fund - UIDP/00674/2020) and Madeira 14-20 Program (Project M1420-01-0145-FEDER-000008, PROEQUIPRAM - *Reforço do Investimento em Equipamentos e Infraestruturas Científicas na RAM*). RS, ARN and MV also acknowledge ARDITI and CQM for their grants ARDITI-CQM-2017-ISG-003, ARDITI-CQM-2017-PDG-011 and ARDITI-CQM-2017-PDG-009, respectively.

[O-08]

Chemical characterization of twelve seized products suspected to contain synthetic cathinones

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[3]Instituto Nacional de Medicina Legal e Ciências Forenses, I.P., Delegação Centro, Largo da Sé Nova, 3000-213 Coimbra, Portugal
[4]Faculdade de Medicina da Universidade de Coimbra, Azinhaga de Santa Comba, Celas, 3000-548 Coimbra, Portugal
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In this study, twelve seized products suspected to contain illicit substances, were analysed by attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), gas chromatography coupled to mass spectrometry (GC-MS), and nuclear magnetic resonance (NMR). Synthetic cathinones were found in all products either as single component or in mixtures. Infrared spectra of all products were consistent with the molecular structure of synthetic cathinones. By GC-MS and NMR analysis, it was possible to identify a total of eight synthetic cathinones namely methedrone, pentedrone, methylone, 3-fluoromethcathinone, *N*-ethylcathinone, buphedrone, α-pyrrolidinohexanophenone (α-PHP), and 4'-methyl-α-pyrrolidinohexanophenone (MPHP). Among the adulterants found in these samples, caffeine and ethylphenidate were the main substances identified. Isopentedrone a by-product of the synthesis of pentedrone was also detected in one seized product. These results highlight the prevalence of synthetic cathinones in seized materials from the Portuguese drug market.

Acknowledgments: This work was supported by FCT - Fundação para a Ciência e a Tecnologia through the CQM Base Fund - UIDB/00674/2020, Programmatic Fund - UIDP/00674/2020, and the Ph.D. scholarships SFRH/BD/116895/2016 and SFRH/BD/117426/2016 granted to João Gonçalves and Vera Alves, respectively, 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).

[O-09]

Piezoelectric PVDF/MWCNTs electrospun nanofibers as a platform for biological applications

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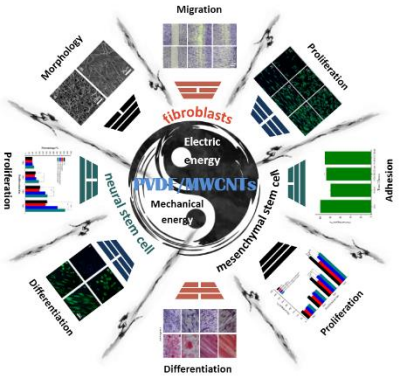
Electrospinning has been widely used to fabricate nanofibers from various kinds of polymers or natural composites. Nowadays, scaffolds made of electrospun nanofibers play critical roles in biological applications. In addition, piezoelectric materials as new smart biomaterials, which exhibit electromechanical behaviour by transforming mechanical energy into electric polarization and vice versa, show great potential in healthcare applications. In our work, we created an inverse piezoelectric stimulation device with interdigitated electrodes coated with electrospun nanofibers made of Polyvinylidene Fluoride (PVDF) and multi-walled carbon nanotubes (MWCNTs), with different alignment. The device was used to explore the effect of mechanical stimulation, created by the inverse piezoelectric nanofibers, on the cells' behaviour. We selected NIH3T3 cells as fibroblasts cell model, PC12 cells as a neural cells model and P3 BMSCs as mesenchymal stem cell model to investigate their cell morphology, proliferation, migration and differentiation. The major contents in our project are presented in graph abstract:



Our results show that the bioactivities of inverse piezoelectric aligned PVDF/MWCNTs nanofibers, hold a great potential on wound healing, nerves regeneration and bone tissue engineering applications.

Acknowledgments: This study was financially supported by Natural Science Foundation of China (81761148028 and 21773026), and Fundamental Research Funds for the Central Universities, 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).

[O-10]

Laponite®-based nanogels for bone tissue regeneration and treatment of osteoporosis

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Osteoporosis is the most prevalent bone illness, being defined by a decrease in bone density that induces greater vulnerability to fractures, often associated with morbidity and loss of independence and, thus, of quality of life. With a growing elderly population, its incidence is predicted to increase in the next decades, along with the costs required for treatments [1].

Bisphosphonates (BPs), such as alendronate, are the most prescribed drugs for its treatment, mainly for their effectiveness and low cost, though they are associated with complex dosage regimens and adverse side effects that can deter patients from correctly following the treatment, displaying also low gastrointestinal absorption and bioavailability [1].

Laponite® is a synthetic clay often used to protect drugs from physiological degradation and has been shown to have osteogenic inducing properties [2]. Thus, Laponite®-based nanogels where alendronate is encapsulated are here proposed as drug delivery systems that will act by reducing osteoclast activity, due to the presence of alendronate, and by promoting osteoblast activity, through the effect of Laponite®.

The nanogels presented high incorporation efficiency of alendronate, a negative zeta potential, and roughly measured 180 nm (a size which drastically increases when the nanogels are frozen and lyophilized, though it returns to close to the initial ones, highlighting the nanogel's restructuring properties). Alendronate was also conjugated to FITC, in order to evaluate the nanogels' kinetics of cellular uptake, which is maximal after 24 hours of incubation, and its internalization pathway, which occurs preferably by macropinocytosis. The nanogels successfully reduced alendronate's cytotoxicity and maintained its hemocompatibility. Importantly, they were effective on osteoblastic differentiation of human mesenchymal stem cells into osteoblasts, inducing *in vitro* bone formation, an effect enhanced by the presence of Laponite®.

Reference: [1] Fazil, M.; Baboota, S.; Sahni, J.K.; Ameeduzzafar, A.J. *Drug Deliv.* **2015**, *22*: 1. [2] Tomás, H.; Alves C.S.; Rodrigues, J. *Nanomed. Nanotechnol. Biol. Med.* **2018**, *14*: 2407.

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[O-11]

The fluorination of poly(amidoamine) (PAMAMG_4-NH_2) dendrimers – synthesis characterization and biological studies

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The incorporation of fluorine in molecules is a strategy used in the development of several drugs since this incorporation, or "fluorination", increases the pharmacokinetic behaviour of the drug as well as improves the protein stability without biological alteration [1,2]. Moreover, biological systems have a lack of fluorine, and this compound is widely used for tracking the behaviour or properties of drugs, cells, and biomacromolecules [1]. Dendrimers are a synthetic polymer broadly used as a delivery system due to their void space, well defined 3D structure, allows the functionalization of their terminal group, among others [3]. Fluorination of dendrimers will improve the serum stability, transfection efficiency, affinity to the cell membrane, and endosomal escape [1,2]. The incorporation of fluorine also enables the use of these systems in magnetic resonance imaging (MRI) [4,5].

In this study, a generation four poly(amidoamine) (PAMAMG_4-NH_2) dendrimer was functionalized with 2,3,5,6-tetrafluoro-4-hydroxybenzoic acid (TFHBA), the fluorinated compound, and 4-hydroxybenzoic acid (HBA), a non-fluorinated compound used as a control due to its resemblance with the fluorinated compound. The synthesis was performed drop wising the solutions with an increased molar equivalent of the compounds into a concentrated PAMAM solution and stirred for two days. This resulted in dendrimers with different functionalization degree of TFHBA and HBA.

The confirmation of the successful conjugation of the compound with the PAMAM dendrimer was done by NMR (*e.g.*, ^{1}H, ^{19}F), FTIR, UV-Visible, fluorescence, and elemental analysis. Biological studies such as cytotoxicity, pDNA condensation capacity, and transfection efficiency were also performed and discussed.

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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). LdO also acknowledges ARDITI for a research grant (ARDITI-CQM/2019/015-BDG).

[O-12]

From fish transforming industry residues to biomaterials: a characterization of hydroxyapatite-based materials extracted from fish by-products

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[2]ISTEC – Institute of Science and Technology for Ceramics, National Research Council (CNR), via Granarolo 64, 48018 Faenza, Italy

The conversion of food industry by-products to compounds with high added value is nowadays a significant topic, for social, environmental, and economic reasons. In this paper, calcium phosphate-based materials were obtained from black scabbardfish (*Aphanopus carbo*) bones and grey triggerfish (*Balistes capriscus*) skin, which are two of the most abundant fish by-products of Madeira Island. Different calcination temperatures between 400 and 1000 °C were employed. Materials obtained from calcination of bones of black scabbard fish were composed by homogeneous mixtures of hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$, HAp) and β-tricalcium phosphate (β-$Ca_3(PO_4)_2$, β-TCP). Because of the high biocompatibility of HAp and the good resorbability of β-TCP, these natural biphasic materials could be very relevant in the field of biomaterials, as bone grafts. The ratio between HAp and β-TCP in the biphasic compound was dependent on the calcination temperature. Differently, the material obtained from skin of grey triggerfish contained HAp as main phase, together with small amounts of other mineral phases, such as halite and rhenanite, which are known to enhance osteogenesis when used as bone substitutes. In both cases, the increase of calcination temperature led to an increase in the particles size with a consequent decrease in their specific surface area. These results demonstrate that from the fish by-products of the most consumed fishes in Madeira Island is possible to obtain bioceramic materials with tunable composition and particle morphology, which could be promising materials for the biomedical field.

Acknowledgments: This work was supported by FCT-Fundação para a Ciência e a Tecnologia (projectPEst-OE/QUI/UI0674/2019, CQM, Portuguese Government funds), and through Madeira 14-20 Program, project PROEQUIPRAM–Reforço do Investimento em Equipamentos e Infraestruturas Científicas na RAM (M1420-01-0145-FEDER-000008) 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). Pedro Ideia is the recipient of a PhD Grant under the project M1420-09-5369-FSE-000001.

[O-13]

Platinum IV complexes conjugated with bis-MPA dendronised PEG: synthesis and characterization

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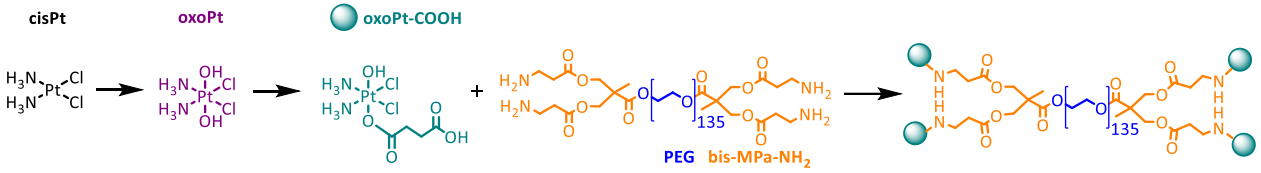
Cisplatin is a chemotherapeutic drug that is commonly used as first-line treatment. Although this drug exhibits a broad spectrum of activity, it is usually associated with drug resistance and severe side effects. To overcome these issues, several platinum-based complexes have been developed over the years (like *carboplatin* and *oxaliplatin*), but they still present most of the problems seen with *cisplatin* [1]. Nanoparticle-based drug formulations are gathering the researchers' attention due to their contribution to improving the therapeutic effect, reducing side effects, and increasing the selectivity of the chemotherapeutics [2]. Polyester dendrimers, such as 2,2-bis(methylol)propionic acid (bis-MPA)-based dendrimers, for instance, are attracting the interest as delivery vehicles since they have been reported as being biodegradable and biocompatible [3, 4].



In this context, the main purpose of this work is to develop a new nanoplatform for the delivery of cis, cis, trans-diammine-dichlorido-dihydroxido-platinum (IV) (oxoplatin) by its conjugation with bis-MPA dendronised polyethylene glycol (PEG) molecules. In this system, the drug is covalently bonded to two bis-MPA dendrons (generation 1) connected in both terminals of a PEG chain (6 kDa). In the first stage, the cisplatin conjugates were synthesized and characterized by mass spectrometry, as well as by NMR and FTIR spectroscopies. Afterwards, further *in vitro* assays will be performed in order to study their degradability and biological behaviour.

References: [1] Hu, X.; Li, F.; Noor, N.; Ling, D. Sci. Bull. **2017**, *62*: 589. [2] Duan, X.; He, C.; Kron, S. J.; Lin, W. *WIREs Nanomed. Nanobiotechnol.* **2016**, *8*: 776. [3] Twibanire, J.-d'A.K.; Grindley, T.B. *Polymers* **2014**, *6*: 179. [4] García-Gallego, S.; Nyström, A.M.; Malkoch, M. *Prog. Polym. Sci.* **2015**, *48*: 85.

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. The Madeira 14-20 Program and 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+ and ARDITI-CQM/2018/007-PDG (Fellowship Grant to MG) are also acknowledged for the support provided.

[O-14]

Rapid screening and analytical characterization of synthetic cannabinoids in 'herbal incenses'

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Frequently marketed as 'synthetic marijuana', synthetic cannabinoids (SCs) have become easily accessible via internet and have been sold as 'herbal incenses'. The substances are added to dried plants or herbs creating the illusion that a natural product is provided. The chemical composition is unknown and is not always the same between brand to brand and from batch to batch. As a result, clinical and forensic toxicology laboratories are continuously confronted with analytical challenges, when dealing with this kind of substances, being of utmost importance to promptly detect and identify SCs in herbal blends with minimal sample preparation and clean up steps.

The present work aims the identification and characterization of nine herbal incenses suspected to contain SCs by GC-MS and NMR techniques.

The analysis of all samples has allowed the initial identification and characterization of 9 SCs, namely JWH-018, JWH-073, JWH-122, JWH-210, AKB-48, XLR-11, MAM-2201, CP47,497-C8 and its enantiomer. Also, it was possible to identify oleamide, vitamin E and vitamin E acetate, three adulterants frequently added to herbal products to mask the active ingredients or added as preservatives. The methodology applied proved to be useful, allowing the preliminary identification of the different SCs in the mixture. Furthermore, the examination of mass spectral fragment ions, as well as the study of both 1D and 2D NMR experiments enabled the characterization of the molecular structure of SCs.

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[O-15]

PAMAM dendrimers - a strategy to improve the efficacy of 1,2-diaminocyclohexane platinum(II)

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Since the discovery of *cisplatin* as an anticancer agent in the early 1970s, various platinum derivatives have been developed, but only a few were clinically approved as chemotherapeutic agents[1]. Among them, that ones with DACH ligand have gain interest in recent years, as a strategy to overcome the resistance regarding cisplatin[2].

In this work, we used a low generation of anionic poly(amidoamine) (PAMAM) dendrimers as a nanocarrier to deliver the 1,2-diaminocyclohexane platinum(II) (DACHPt), active part of oxaliplatin, into tumor cells, by expecting to increase its efficacy as an anticancer agent.

The prepared metallodendrimers were characterized by different technics, including NMR, FTIR, UV-Visible/Fluorescence Spectroscopy, and Zeta-potential. Their effectiveness was then studied in different cancer cell lines(*e.g.*, A2780, A2780CisR, MCF-7, CACO-2, and in the BJ normal cell line), and the IC50 was also determined. The metallodendrimer G2.5(COO(DACHPt))$_{16}$ with better efficacy was used to encapsulate the 5-Fluorouracil (5-FU), an anticancer drug also used in cancer treatment of, for instance, colon and breast cancer. The capability to release the drug is being studied *in vitro* in PBS at pH 5 and 7.4 (37°C).

Afterward, the anticancer activity of the nanosystem will be evaluated through the synergetic effect of our approach regarding resistance to cancer cells.

References: [1] Desoize, B. *Anticancer Res.* **2004**, *24*: 1529. [2] Raymond, E.; Chaney, S.G.; Taamma, A.; Cvitkovic, E. *Ann. Oncol.* **1998**, *9*: 1053.

Acknowledgments: This work was supported by Fundação para a Ciência e a Tecnologia (Base Fund UIDB/00674/2020 and Programmatic Fund UIDP/00674/2020, Portuguese Government Funds), 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 PhD Grant project M1420-09-5369-FSE-000001 (CC).

[O-16]

Exploring the controlled growth of copper-based nanoparticles

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Copper-based nanoparticles (CuNPs) are particularly appealing materials for the replacement of more expensive and less earth-abundant metals such as silver and gold, which are used in several commercial processes. Cu also displays good electronic, antimicrobial, optical, and chemical properties despite its limitations under atmospheric conditions (*e.g.,* CuNPs are intrinsically prone to oxidation). Various efforts have been made to increase the stability of CuNPs, including the association of CuNPs with organic structures [1].

To prepare and characterize long-term stable Cu-based NPs, hydroxyl-terminated polyamidoamine (PAMAM) dendrimer was used as a template for the controlled growth of the CuNPs. Several reaction parameters were tested, mainly pH, reducing agents, and Cu and PAMAM concentrations.

The final product, as well the starting and intermediate compounds, were studied using various characterization techniques, which include: Ultraviolet-Visible (UV-Vis) and Nuclear Magnetic Resonance (NMR) Spectroscopy, as well as Scanning Electron Microscopy (SEM).

Complementary studies and characterization are still needed to overcome the stabilization of the particles at the nanoscale and confirm the chemical nature of the final product.

References: [1] Din, M.I. & Rehan, R. *Anal. Lett.* **2017**, *50*: 50.

Acknowledgments: This work was suported by the FCT - Fundação para a Ciência e a Tecnologia through the CQM Strategic Project PEst-OE/QUI/UI0674/2019, CQM Base Fund - UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020, and by the 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). DF and CSA also acknowledge the ARDITI for a research grant (ARDITI-CQM-2019-007-MDG) and a Post-doc Grant (002458/2015/132), respectively.

[O-17]

Electroactive polymer-metal composite fibres

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Electrospinning is a cost-efficient technique to prepare ultra-thin polymeric fibres, which can be easily employed in the laboratory and scaled up to an industrial process [1]. In this work, we have prepared reproducible particle-electrospun fibre composites using polyvinylidene fluoride (PVDF), a non-reactive hydrophobic piezoelectric polymer [2], combined with copper or silver particles following six different strategies [3].

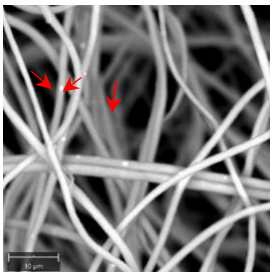

Figure 1. Silver particles incorporated in PVDF electrospun fibres structure

Fibres and particles with diameters below 1000 nm were obtained with polymer-metal composite fibres average porosities of 60 - 100 nm. The formation of the electroactive phase responsible for the piezoelectric response was also confirmed.

The preliminary characterization of the prepared composites envisages the application of this electroactive material as a filter to capture aerosolised particles in the range from 60 to 400 nm [4] and for the separation of viruses from other microorganisms [5]. Since both Ag and Cu particles have a known antimicrobial activity [6] and the PVDF crystallize in different polymorphisms [7], the range of applications is potentially even broader.

References: [1] Ji, W.; Sun, Y.; Yang, F.; van den Beucken, J.J.J.P.; Fan, M.; Chen, Z.; Jansen, J.A. *Pharm. Res.* **2011**, *28*: 1259. [2] Abbasipour,·M.; Khajavi, R.; Yousefi, A.A.; Yazdanshenas, M.E.; Razaghian, F. *J. Mater. Sci. Mater. Electron.* **2017**, *28*: 15942. [3] a) Xue, J.; Wu, T.; Dai, Y.; Xia, Y. *Chem. Rev.* **2019**, *119*: 5298; b) P-Santos, I.; Liz-Marzán, L.M. *Langmuir* **1999**, *15*: 948. [4] Leung, W.W-F.; Sun, Q. *Sep. Purif. Technol.* **2020**, *245*: 116887. [5] Moce ´ -Llivina, L.; Jofre, J.; Muniesa, M. *J. Virol. Methods* **2003**, *109*: 99. [6] a) Hong, K.H.; Park, J.L.; Sul, I.H.; Youk, J.H.; Kang, T.J. *J. Polym. Sci. B Polym. Phys.* **2006**, *44*: 2468; b) Din, M.I. & Rehan, R. *Anal. Lett.* **2017**, *50*: 50. [7] Abolhasani, M.M.; Azimia, S.; Fashandib, H. *RSC Adv.* **2015**, *5*: 61277.

Acknowledgments: The authors acknowledge the funds from FCT - Fundação para a Ciência e a Tecnologia (CQM Base Fund - UIDB/00674/2020, and Programmatic Fund - UIDP/00674/2020) and ARDITI - Agência Regional para o Desenvolvimento da Investigação, Tecnologia e Inovação (M1420-01-0145-FEDER-000005 - Centro de Química da Madeira - CQM+). Also, CCM and DF thank the grants ARDITI-CQM/2019/001-STMG-SEM and ARDITI-CQM-2019-007-MDG, respectively.

[O-18]

Metabolic profile of cells in the presence of cinnamic acid-terminated dendrimers

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Alpha-cyano-4-hydroxycinnamic acid (ACCA) displays *in vitro* and *in vivo* efficacy against the reprogramming of glucose metabolism that most cancer cells suffer via the "Warburg effect" [1,2]. Recently, ACCA was used as a targeting group in nanoparticles for targeted cancer therapy and to avoid oxidative stress [3]. One of the nanomaterials most explored in the field of cancer are dendrimers since they can be easily functionalized [4]. The goal of this work was to synthetize and characterize new cinnamic acid-terminated dendrimers, evaluate their cytocompatibility, and study their influence on cancer metabolism by ^{1}H NMR metabolomics. Poly(amidoamine) (PAMAM) dendrimers generation 4 were functionalized with ACCA by a carbodiimide reaction. The characterization by NMR, IV, UV-Visible spectroscopy, elemental analysis, and MALDI-TOF-MS indicates that the product obtained had 48 ACCA molecules linked per dendrimer. The cytotoxicity was evaluated in the CAL-72 cell line by the resazurin assay for 24h. After functionalization, the dendrimer shows 3 times less cytotoxicity. The ^{1}H NMR metabolomics experiments were done using treated and untreated cell extracts (the pristine and the functionalized dendrimer were analyzed). Statistical analysis showed that assays with the pristine dendrimers exhibited higher discrimination between treated and non-treated cells in comparison with the functionalized ones. Pathway analysis was also performed using the Metaboanalyst webserver to identify which metabolic pathways are influenced by the nanomaterial treatment. Results demonstrated that functionalization with the ACCA made the dendrimer more cytocompatible. The cinnamic acid-based nanomaterials show the potential to be more selective, presenting fewer collateral effects to be used in novel drug delivery systems.

References: [1] Hanahan, D.; Weinberg, R.A. *Cell* **2011**, *144*: 646. [2] Gurrapu, S.; Jonnalagadda, S.K.; Alam, M.A.; Nelson, G.L.; Sneve, M.G.; Drewes, L.R.; Mereddy, V.R. *ACS Med. Chem. Lett.* **2015**, *6*: 558. [3] Caloria, I.R.; Piva, H.L.; Tedesco, A.C. *J. Drug Delivery Sci. Technol.* **2020**, *57*: 101633. [4] Leiro, V.; Garcia, J.P.; Tomás, H.; Pêgo, A.P. *Bioconj. Chem.* **2015**, *26*: 1182.

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[O-19]

Novel dendrimer-based nanoparticles for targeted computed tomography imaging of cancer cells

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Despite advances in clinical treatment, developments in early-stage cancer diagnosis are shortcoming. Conventional imaging techniques as X-ray Computed Tomography (CT) rely on the use of toxic agents with a short circulation time (*e.g.,* Iodine). Here, gold nanoparticles (AuNPs) have displayed the potential to be used in cancer imaging due to their higher X-ray attenuation coefficient leading to contrast enhancement [1]. Polyamidoamine (PAMAM) dendrimers are considered promising candidates for diagnostic, imaging, and drug delivery applications due to their unique structural properties (*e.g.,* internal cavities, easily modifiable surface functionality), which allow for the conjugation of drugs, targeting molecules and/or imaging agents [2].

Aiming at the development of a new system for targeted X-ray CT imaging of CD44 overexpressing cancer cells, hyaluronic acid (HA), a naturally occurring glycosaminoglycan often used as a drug carrier and targeting ligand for CD44 receptors [3], was conjugated to amine-terminated generation 5 PAMAM dendrimers (G5.NH_2). The conjugate acted as a template for the synthesis of dendrimer-entrapped gold nanoparticles (Au DENPs). Characterization results of the HA-modified dendrimers and their respective Au DENPs were obtained by ^{1}H and ^{13}C NMR spectroscopy, FTIR spectroscopy, dynamic light scattering, zeta potential, and UV-Vis spectroscopy. Preliminary data shows the successful conjugation of HA to the terminal groups of the PAMAM dendrimer. The presence of Au DENPs was also confirmed by UV-Vis.

References: [1] Mutalib, S.A.; Ristaniah; Anwar, E.; Radji, M.; Pujiyanto, A.; Purnamasari P.; Joshita D.; Adang, H.G. *Macromol. Symp.* **2015**, *353*: 96. [2] Biricova, V.; Laznickova, A. *Bioorg. Chem.* **2009**, *37*: 185. [3] Plattt, V.M.; Szoka, F.C. *Mol. Pharmaceut.* **2008**, *5*: 474.

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[O-20]

Surface modification of carbon dots with 4-aminobenzonitrile through amide coupling reaction

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Carbon dots (CDs) are emergent zero-dimensional nanomaterials, with sizes ranging between 2-20 nm that are photoluminescent, water-soluble, and low cytotoxic [1]. The photoluminescent properties are related with the surface groups of carbon dots, and hydroxy, carboxy, and amino groups are normally encountered [2]. The surface functionalization of carbon dots can be achieved by covalent methods *e.g.* through amide coupling reaction [3]. Carbodiimide agents such as EDC and DCC are commonly used, and DCC (N,N'-Dicyclohexylcarbodiimide) was selected as intermediate for the covalent bonding between carboxyl-CDs and 4-aminobenzonitrile.

In this work, the surface of carboxyl-CDs was modified by amide coupling reaction. First, the carboxyl-CDs were synthesized by hydrothermal synthesis, using ascorbic acid as starting material. The formation of carbon dots were confirmed by AFM, UV-Vis and Fluorescence spectroscopy, NMR, Infrared, and DLS. Then, to synthesize CDs@4-aminobenzonitrile, the carboxyl-CDs were combined with DCC-carbodiimide and 4-aminobenzonitrile, and the reaction was carried at room-temperature and protected from light. The CDs@4-aminobenzonitrile were characterized by UV-Vis and Fluorescence Spectroscopy, NMR, and DLS, which helped to confirm the carbon dots surface modification. All these results will be presented and discussed.

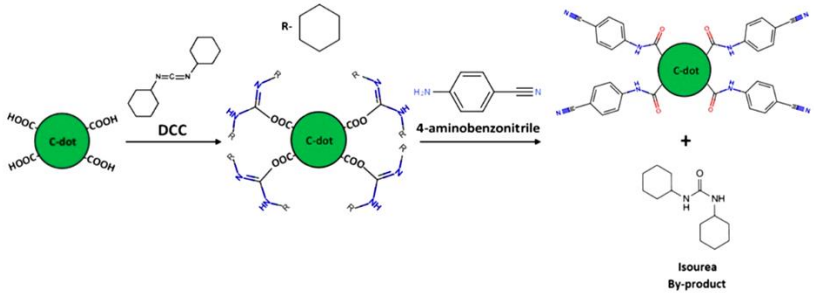

Figure 1. Strategy for the synthesis of CDs@4-aminobenzonitrile.

References: [1] Kozák, O.; Sudolská, M.; Pramanik, G.; Cígler, P.; Otyepka, M.; Zboril, R.; *Chem. Mat.* **2016**, *28*: 4085. [2] Cayuela, A.; Soriano, M.L.; Carrillo-Carrión, C.; Valcárcel, M. *Chem. Commun*. **2016**, *52*: 1311. [3] Yan, F.; Jiang, Y.; Sun, X.; Bai, Z.; Zhang, Y.; Zhou, X. *Microchim. Acta* **2018**, *185*: 424.

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[O-21]

Development of bacteriophage-based bionanosensors for the diagnosis of infectious diseases using the phage display technique

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Zika is an infectious viral disease, which had a recent worldwide outbreak. This illness is caused by the Zika virus (ZIKV), a flavivirus transmitted by the *Aedes aegypti* mosquito. Presently, there is still no treatment for Zika infection and no vaccine to prevent it. As to the current diagnostic tools, they are time-consuming methods that require expensive and specialized laboratory equipment, and present low specificity [1]. Since a routine and accurate assay for the diagnosis of Zika infection is still not currently available, the aim of this project is the development of an approach, based on the phage display technology, that will allow for an early, rapid and differential routine diagnosis of Zika.

The phage display technology is based on the presentation of randomized peptide sequences on the surface of bacteriophages, which can be used for the affinity screening of specific target molecules. In this technique, a gene encoding a protein of interest is inserted into a phage coat protein gene, causing the bacteriophage to display the protein on its outside while containing the gene for the protein in its inside [2]. This technology utilizes 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 disease target molecules with high sensitivity and selectivity. The target-bound bacteriophages are amplified, and the correspondent Zika-specific peptides identified and characterized.

During this project, a commercially available phage-displayed peptide library was screened against a specific antibody for Zika, in order to identify the peptides that specifically recognized the disease target molecules. Our main aim is to use these phage-displayed peptides in the development of bionanosensors, which will work as sensitive viral detection and serotyping tools. This type of innovative biosensing method will allow for a non-invasive, rapid, and in real time diagnosis of the disease.

Reference: [1] Peters, R.; Stevenson, M. *Clin. Microbiol. Infect.* **2019**, *25*: 142. [2] Bazan, J.; Calkosinski, I.; Gamian, A. *Hum Vaccin Immunother* **2012**, *8*: 1817.

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The Post-Doc Grant ARDITI-CQM-2017-009-PDG (MV) and the Bachelor Research Grant ARDITI-CQM-2019-015-BDG (HC) are also acknowledged.

[O-22]

Unveiling the mechanism of action of novel anticancer candidates – $[Ru(\eta^5\text{-}C_5H_5)(PPh_3)_2]$-PAMAM metallodendrimers

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Ruthenium complexes represent an interesting alternative to platinum drugs as attractive candidates against tumors with acquired drug resistance, with the ability to follow a multitargeted approach [1,2]. They not only target DNA but can also exploit the iron-transporter protein transferrin to facilitate their uptake into tumor cells [3]. Furthermore, their therapeutic activity, solubility, and selectivity can be enhanced when functionalized on dendrimers' periphery, producing metallodendrimers [4]. Based on our knowledge on the field [5] we herein present the synthesis and characterization (by NMR, FTIR, EA, MS, and DLS techniques) of a new family of ruthenium(II)-metallodendrimers from the zero to the third generation (4 to 32 Ru-moieties, respectively) based on polynitrile PAMAM dendritic scaffolds quantitatively coordinated to the metallofragment $[Ru(\eta_5\text{-}C_5H_5)(PPh_3)_2]^+$. It's in vitro cytotoxicity, hemolytic activity, and reactivity towards DNA were also evaluated.

These compounds revealed to be promising anticancer candidates against the studied cancer cell lines (A2780, A2870cisR, and MCF-7), with an IC50 at a nanomolar range, when compared with the organometallic scaffold $RuCp(PPh_3)_2Cl$ (RuCp) and cisplatin; exhibiting non-toxicity for the healthy human red blood cells and strong interactions with calf thymus DNA. Further biological studies to disclose the mechanism of action of the G3-metallodendrimer when compared with RuCp and cisplatin were investigated by flow cytometry in the breast cancer cell line MCF-7: mechanism of cell death by apoptosis/necrosis, autophagy, and generation of excessive levels of intracellular reactive oxygen species (ROS); cytostatic potential and the ability to induce the loss of mitochondrial membrane potential (JC-1 assay). Optimized reproducible studies revealed that the G3-metallodendrimer led to cell death by higher levels of late apoptosis, necrosis, and ROS generation, and induced cell cycle arrest in the G0/G1 phase.

References: [1] Zeng, L.; Gupta, P.; Chen, Y.; Wang, E.; Ji, L.; Chao, H.; Chen, Z-S. *Chem. Soc. Rev.* **2017**, *46*: 5771. [2] Kenny, R.G.; Marmion, C.J. *Chem. Rev.* **2019**, *119*: 1058. [3] Boros, E.; Dyson, P.J.; Gasser, G. *Chem.* **2020**, *6*: 41. [4] Govender, P.; Therrien, B.; Smith, G.S. *Eur. J. Inorg. Chem.* **2012**, *17*: 2853. [5] Gouveia, M.; Figueira, J.; Jardim, M.G.; Castro, R.; Tomás, H.; Rissanen, K.; Rodrigues, J. *Molecules* **2018**, *23*: 1471.

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7TH CQM ANNUAL MEETING

CQM CENTRO DE QUÍMICA DA MADEIRA

Publications 2019/20

Publications 2019

- **1. Serina, J.**; **Fernandes, M. X.**; **Castilho, P. C.** Effects of hydroxycinnamic acids on the glycolysis pathway *S. Afr. J. Bot.* **2019**, *120*, 219-229. (IF: **1.442**) Q2 (Plant Science)
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- **4.** Casado, N.; Morante-Zarcero, S.; Pérez-Quintanilla, D.; **Câmara, J. d. S.**; Sierra, I. Dispersive Solid-Phase Extraction of Polyphenols from Juice and Smoothie Samples Using Hybrid Mesostructured Silica Followed by Ultra-high-Performance Liquid Chromatography-Ion-Trap Tandem Mass Spectrometry *Journal of Agricultural and Food Chemistry* **2019**, *67*, 955-967. (IF: **3.571**) Q1 (Chemistry)
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- **8. Medina, S.**; **Perestrelo, R.**; **Silva, P.**; **Pereira, J. A.M.**; **Câmara, J. S.** Current trends and recent advances on food authenticity technologies and chemometric approaches *Trends Food Sci. Technol.* **2019**, *85*, 163-176. (IF: **6.609**) Q1 (Food Science)
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- **14.** Milenkovic, I.; **Algarra, M.**; Alcoholado, C.; Cifuentes, M.; Lázaro-Martínez, J. M.; Rodríguez-Castellón, E.; Mutavdžić, D.; Radotić, K.; Bandosz, T. J. Fingerprint imaging using N-doped carbon dots *Carbon* **2019**, *144*, 791-797. (IF: **7.082**) Q1 (Chemistry)
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- **23. Silva, C.**; **Perestrelo, R.**; **Silva, P.**; Capelinha, F.; **Tomás, H.**; **Câmara, J. S.** Volatomic pattern of breast cancer and cancer-free tissues as a powerful strategy to identify potential biomarkers *Analyst* **2019**, *144*, 4153-4161. (IF: **4.019**) Q1 (Analytical Chemistry)
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- **28. Ideia, P.**; **Pinto, J.**; **Ferreira, R.**; **Figueiredo, L.**; **Spínola, V.**; **Castilho, P. C. M. F.** Fish Processing Industry Residues: A Review of Valuable Products Extraction and Characterization Methods *Waste Biomass Valorization* **2019**, 1-24. (IF: **2.358**) Q2 (Waste Management and Disposal)
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- **30.** Qiu, J.; Hameau, A.; **Shi, X.**; **Mignani, S. M.**; Majoral, J. P.; Caminade, A. M. Fluorescent Phosphorus Dendrimers: Towards Material and Biological Applications *ChemPlusChem* **2019**, *84*, 1070-1080. (IF: **3.441**) Q1 (Chemistry)
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- **33.** Qiao, Z.; Wu, Y.; Tang, B.; **Perestrelo, R.**; Bhalla, R. An AIE and ESIPT active Schiff base as colorimetric probe of Fe3+ and turn-on fluorescent probe of Al3+: Experimental and theoretical studies *Tetrahedron Lett.* **2019**, *60*, 150918-. (IF: **2.259**) Q2 (Organic Chemistry)
- **34.** Wu, J.; Su, D.; Qin, C.; Li, W.; **Rodrigues, J. M. C.**; **Sheng, R.**; Zeng, L. A fast responsive chromogenic and near-infrared fluorescence lighting-up probe for visual detection of toxic thiophenol in environmental water and living cells *Talanta* **2019**, *201*, 111-118. (IF: **4.916**) Q1 (Analytical Chemistry)
- **35. Perestrelo, R.**; **Silva, C.**; **Câmara, J. d. S.** Madeira Wine Volatile Profile. A Platform to Establish Madeira Wine Aroma Descriptors *Molecules* **2019**, *24*, 3028-. (IF: **3.060**) Q2 (Analytical Chemistry)
- **36.** Sampaio-Dias, I. E.; Silva-Reis, S. C.; García-Mera, X.; Brea, J.; Loza, M. I.; **Alves, C. S.**; **Algarra, M.**; Rodríguez-Borges, J. E. Synthesis, Pharmacological, and Biological Evaluation of MIF-1 Picolinoyl Peptidomimetics as Positive Allosteric Modulators of D2R *ACS Chem. Neurosci.* **2019**, *10*, 3690-3702. (IF: **3.861**) Q1 (Biochemistry)
- **37.** Hamed, O.; Lail, B.A.; Deghles, A.; Qasem, B.; Azzaoui, K.; Obied, A. A.; **Algarra, M.**; Jodeh, S. Synthesis of a cross-linked cellulose-based amine polymer and its application in wastewater purification *Environ. Sci. Pollut. Res.* **2019**, *26*, 28080-28091. (IF: **2.914**) Q2 (Environmental Chemistry)
- **38.** Wu, X.; Zeng, L.; Chen, B. Q.; Zhang, M.; **Rodrigues, J. M. C.**; **Sheng, R.**; Bao, G. M. A selective cascade reaction-based probe for colorimetric and ratiometric fluorescence detection of benzoyl peroxide in food and living cells *J. Mat. Chem. B* **2019**, *7*, 5775-5781. (IF: **5.047**) Q1 (Biochemistry)
- **39. Perestrelo, R.**; **Silva, P.**; **Porto-Figueira, P.**; **Pereira, J. A. M.**; **Silva, C.**; **Medina, S.**; **Câmara, J. S.** QuEChERS - Fundamentals, relevant improvements, applications and future trends *Anal. Chim. Acta* **2019**, *1070*, 1-28. (IF: **5.123**) Q1 (Analytical Chemistry)
- **40.** Li, A.; Fan, Y.; Cao, X.; Chen, L.; Wang, L.; **Alves, C. S.**; **Mignani, S. M.**; Majoral, J. P.; **Tomás, H.** ; **Shi, X.** Morpholino-functionalized phosphorus dendrimers for precision regenerative medicine: osteogenic differentiation of mesenchymal stem cells *Nanoscale* **2019**, *11*, 17230-17234. (IF: **6.970**) Q1 (Materials Science)

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- **42.** Sevilla, R.; Herrero, M.; Alonso, B.; García-Armada, M. P.; **Algarra, M.**; Casado, C. M. Synthesis, characterization and electrochemical behaviour of dimethyleneamine-bridged methylated and non-methylated biferrocenyl derivatives *J. Organomet. Chem.* **2019**, *896*, 183-187. (IF: **2.066**) Q2 (Inorganic Chemistry)
- **43.** Casado, N.; **Perestrelo, R.**; **Silva, C. L.**; Sierra, I.; **Câmara, J. S.** Comparison of high-throughput microextraction techniques, MEPS and μ-SPEed, for the determination of polyphenols in baby food by ultrahigh pressure liquid chromatography *Food Chem.* **2019**, *292*, 14-23. (IF: **4.946**) Q1 (Food Science)
- **44. Majoral, J.-P.**; Zablocka, M.; Koprowski, M.; Hameau, A.; **Shi, X.**; **Mignani, S. M.**; Caminade, A.-M. Design, complexing and catalytic properties of phosphorus thiazoles and benzothiazoles: a concise overview *New J. Chem.* **2019**, *43*, 16785-16795. (IF: **3.069**) Q1 (Materials Chemistry)
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- **47.** Xiong, Z.; **Alves, C. S.**; Wang, J.; Li, A.; Liu, J.; Shen, M.; **Rodrigues, J. M. C.**; **Tomás, H.** ; **Shi, X.** Zwitterion-functionalized dendrimer-entrapped gold nanoparticles for serum-enhanced gene delivery to inhibit cancer cell metastasis *Acta Biomater.* **2019**, *99*, 320-329. (IF: **6.638**) Q1 (Biomaterials)
- **48.** Chen, L.; **Mignani, S. M.**; Caminade, A. M.; Majoral, J. P. Metal-based phosphorus dendrimers as novel nanotherapeutic strategies to tackle cancers: A concise overview *Wiley Interdiscip. Rev.-Nanomed. Nanobiotechnol.* **2019**, *11*, e1577-. (IF: **6.140**) Q1 (Nanoscience and Nanotechnology)
- **49. Medina, S.**; **Perestrelo, R.**; **Santos, R.**; Pereira, R.; **Câmara, J. d. S.** Differential volatile organic compounds signatures of apple juices from Madeira Island according to variety and geographical origin *Microchem J.* **2019**, *150*, 104094-104104. (IF: **3.206**) Q2 (Analytical Chemistry)
- **50.** Milenkovic, I.; Mitrović, A.; **Algarra, M.**; Lázaro-Martínez, J. M.; Rodríguez-Castellón, E.; Maksimović, V.; Spasić, S. Z.; Beškoski, V. P.; Radotić, K. Interaction of Carbohydrate Coated Cerium-Oxide Nanoparticles with Wheat and Pea: Stress Induction Potential and Effect on Development *Plants-Basel* **2019**, *8*, 478-. (IF: **2.632**) Q1 (Plant Science)
- **51. Silva, L. Catarina**; **Silva, C. G. S. L.**; **Perestrelo, R. M. d. S.**; **Silva, P.**; **Tomás, H.** ; **Câmara, J. d. S.** Untargeted Urinary 1H NMR-Based Metabolomic Pattern as a Potential Platform in Breast Cancer Detection *Metabolites* **2019**, *9*, 269-. (IF: **3.303**) Q2 (Biochemistry)
- **52. Zou, Y.**; Li, D.; Shen, M.; **Shi, X.** Polyethylenimine-Based Nanogels for Biomedical Applications *Macromol. Biosci.* **2019**, *19*, 1900272-. (IF: **2.895**) Q1 (Materials Chemistry)
- **53. Perestrelo, R. M. d. S.**; **Silva, C. G. S. L.**; Fernandes, X. M.; **Câmara, J. d. S.** Prediction of Terpenoid Toxicity Based on a Quantitative Structure–Activity Relationship Model *Foods* **2019**, *8*, 628-. (IF: **3.011**) Q2 (Food Science)
- **54.** Zhu, W.; Zhao, L.; Fan, Y.; Zhao, J.; **Shi, X.**; Shen, M. 131I-Labeled Multifunctional Polyphosphazene Nanospheres for SPECT Imaging-Guided Radiotherapy of Tumors *Adv. Healthc. Mater.* **2019**, *8*, 1901299-. (IF: **6.270**) Q1 (Biomaterials)

Publications 2020 (ongoing)

- **1. Spínola, V.**; Llorent-Martínez, E. J.; **Castilho, P. C. M. F.** Inhibition of α-amylase, α-glucosidase and pancreatic lipase by phenolic compounds of Rumex maderensis (Madeira sorrel). Influence of simulated gastrointestinal digestion on hyperglycaemia-related damage linked with aldose reductase activity and protein g . *LWT-Food Sci. Technol.* **2020**, *118*, 108727-. (IF: **3.714**) Q1 (Food Science)
- **2.** Li, A.; Qiu, J.; Zhou, B.; Xu, B.; Xiong, Z.; Hao, X.; **Shi, X.**; Cao, X. The gene transfection and endocytic uptake pathways mediated by PEGylated PEI-entrapped gold nanoparticles . *Arab. J. Chem.* **2020**, *13*, 2558-2567. (IF: **3.298**) Q1 (Chemistry)
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- **4. Pinto, D.**; Amaro, A. M.; Bernardo, L. Experimental Study on the Surface Properties of Nanoalumina-Filled Epoxy Resin Nanocomposites . *Appl. Sci.-Basel* **2020**, *10*, 733-. (IF: **2.217**) Q2 (Materials Science)
- **5.** Placines, C.; Castañeda-Loaiza, V.; Rodrigues, M. J.; Pereira, C. G.; Stefanucci, A.; Mollica, A.; Zengin, G.; Llorent-Martínez, E. J.; **Castilho, P. C. M. F.**; Custódio, L. Phenolic Profile, Toxicity, Enzyme Inhibition, In Silico Studies, and Antioxidant Properties of Cakile maritima Scop. (Brassicaceae) from Southern Portugal . *Plants-Basel* **2020**, *9*, 142-. (IF: **2.762**) Q1 (Plant Science)
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- **9.** Zhang, C.; Sun, W.; Wang, Y.; Xu, F.; Qu, J.; Xia, J.; Shen, M.; **Shi, X.** Gd-/CuS-Loaded Functional Nanogels for MR/PA Imaging-Guided Tumor-Targeted Photothermal Therapy . *ACS Appl. Mater. Interfaces* **2020**, *12*, 9107-9117. (IF: **8.456**) Q1 (Medicine)
- **10. Algarra, M.**; Moreno, V.; Lázaro-Martínez, J. M.; Rodríguez-Castellón, E.; Soto, J.; Morales, J.; Benítez, A. Insights into the formation of N doped 3D-graphene quantum dots. Spectroscopic and computational approach . *J. Colloid Interface Sci.* **2020**, *561*, 678-686. (IF: **6.361**) Q1 (Biomaterials)
- **11. Perestrelo, R. M. d. S.**; **Bordiga, Matteo**; Locatelli, M.; **Silva, C. G. S. L.**; **Câmara, J. d. S.** Polyphenols, biogenic amines and amino acids patterns in Verdelho wines according to vintage . *Microchem J.* **2020**, *153*, 104383-. (IF: **3.206**) Q2 (Analytical Chemistry)
- **12.** Quintana, G.; **Spínola, V.**; **Martins, G. N.**; Gerbino, E.; Gomez-Zavaglia, A.; **Castilho, P. C. M. F.** Release of health-related compounds during in vitro gastro-intestinal digestion of okara and okara fermented with Lactobacillus plantarum . *Journal of Food Science and Technology* **2020**, *57*, 1061-1070. (IF: **1.850**) Q1 (Food Science)
- **13.** Chen, L.; Fan, Y.; Qiu, J.; Laurent, R.; Li, J.; Bignon, J.; **Mignani, S. M.**; Caminade, A.-M.; **Shi, X.**; Majoral, J.-P. Potent anticancer efficacy of first-in-class Cu(II) and Au(III) metaled phosphorus dendrons with distinct cell death pathways . *Chem.-Eur. J.* **2020**, 1-. (IF: **5.160**) Q1 (Chemistry)

- **14. Algarra, M.**; Soto, J.; Silva, L. P.; Pino-González, M. S.; Rodríguez-Borges, J. E.; Mascetti, J.; Borget, F.; Reisi-Vanani, A.; Luque, R. Insights into the Photodecomposition of Azidomethyl Methyl Sulfide: A S2/S1 Conical Intersection on Nitrene Potential Energy Surfaces Leading to the Formation of S-Methyl-N-sulfenylmethanimine . *J. Phys. Chem. A* **2020**, *124*, 1911-1921. (IF: **2.641**) Q1 (Physical and Theoretical Chemistry)
- **15. Freitas, J.**; Vaz-Pires, P.; **Câmara, J. d. S.** From aquaculture production to consumption: Freshness, safety, traceability and authentication, the four pillars of quality . *Aquaculture* **2020**, *518*, 734857-. (IF: **3.022**) Q1 (Aquatic Science)
- **16.** An, F.; Yang, Z.; Zheng, M.; Mei, T.; Deng, G.; Guo, P.; Li, Y.; **Sheng, R.** Rationally assembled albumin/indocyanine green nanocomplex for enhanced tumor imaging to guide photothermal therapy . *J. Nanobiotechnol.* **2020**, *18*, 49-. (IF: **5.345**) Q1 (Biomedical Engineering)
- **17. Perestrelo, R. M. d. S.**; **Câmara, J. d. S.** Chemical/Instrumental Approaches to the Evaluation of Wine Chemistry . *Molecules* **2020**, *25*, 1363-. (IF: **3.060**) Q1 (Chemistry)
- **18. Fernandes, S.**; **Gois, A.**; **Mendes, F.**; **Perestrelo, R. M. d. S.**; **Medina, S.**; **Câmara, J. d. S.** Typicality Assessment of Onions (Allium cepa) from Different Geographical Regions Based on the Volatile Signature and Chemometric Tools . *Foods* **2020**, *9*, 375-. (IF: **4.092**) Q2 (Food Science)
- **19.** Xiao, T.; Qin, J.; Peng, C.; Guo, R.; Lu, X.; **Shi, X.** A Dendrimer-Based Dual Radiodense Element-Containing Nanoplatform for Targeted Enhanced Tumor Computed Tomography Imaging . *Langmuir* **2020**, *36*, 3096-3103. (IF: **3.683**) Q1 (Materials Science)
- **20. Pinto, D. G.**; **Rodrigues, J. M. C.**; Bernardo, L. A Review on Thermoplastic or Thermosetting Polymeric Matrices Used in Polymeric Composites Manufactured with Banana Fibers from the Pseudostem . *Appl. Sci.-Basel* **2020**, *10*, 3023-. (IF: **2.474**) Q1 (Engineering)
- **21.** Chen, L.; Li, J.; Fan, Y.; Qiu, J.; Cao, L.; Laurent, R.; **Mignani, S. M.**; Caminade, A.-M.; Majoral, J.-P.; **Shi, X.** Revisiting Cationic Phosphorus Dendrimers as a Nonviral Vector for Optimized Gene Delivery Toward Cancer Therapy Applications . *Biomacromolecules* **2020**, *21*, 2502-2511. (IF: **6.092**) Q1 (Biomaterials)
- **22.** Sendão, R.; Yuso, M. V. M. Y.; **Algarra, M.**; Silva, J. C. G. E.; Silva, L. P. Comparative life cycle assessment of bottom-up synthesis routes for carbon dots derived from citric acid and urea . *J. Clean Prod.* **2020**, *254*, 120080-. (IF: **6.395**) Q1 (Environmental Science)
- **23. Freitas, P. D. I.**; **Sousa-Ferreira, I.**; **Castilho, P. C. M. F.** A Novel and Simpler Alkaline Hydrolysis Methodology for Extraction of Ferulic Acid from Brewer's Spent Grain and its (Partial) Purification through Adsorption in a Synthetic Resin . *Foods* **2020**, *9*, 600-. (IF: **3.011**) Q2 (Food Science)
- **24.** Bonet-San-Emeterio, M.; **Algarra, M.**; **Petkovic, M.**; Valle, M. Modification of electrodes with N- and S-doped carbon dots. Evaluation of the electrochemical response . *Talanta* **2020**, *212*, 120806-. (IF: **4.916**) Q1 (Analytical Chemistry)
- **25. Mignani, S. M.**; **Shi, X.**; Ceña, V.; Majoral, J.-P. Dendrimer- and polymeric nanoparticle-aptamer bioconjugates as nonviral delivery systems: a new approach in medicine . *Drug Discov. Today* **2020**, *25*, 1065-1073. (IF: **7.321**) Q1 (Drug Discovery)
- **26. Martins, G. N. G.**; **Spínola, V.**; **Castilho, P. C. M. F.** Release of adsorbed ferulic acid in simulated gastrointestinal conditions . *Eur. Food Res. Technol.* **2020**, *246*, 1297-1306. (IF: **2.366**) Q2 (Food Science)
- **27.** Garrido, A.; Lepailleur, A.; **Mignani, S. M.**; Dallemagne, P.; Rochais, C. hERG toxicity assessment: Useful guidelines for drug design . *Eur. J. Med. Chem.* **2020**, *195*, 112290-. (IF: **5.572**) Q1 (Drug Discovery)
- **28. Câmara, J. d. S.**; Lourenço, S.; **Silva, C. G. S. L.**; Lopes, A.; Andrade, C.; **Perestrelo, R. M. d. S.** Exploring the potential of wine industry by-products as source of additives to improve the quality of aquafeed . *Microchemical J.* **2020**, *155*, 104758-. (IF: **3.206**) Q2 (Analytical Chemistry)

- **29.** Wang, Z.; Zhang, X.; Lin, Q.; Sun, J.; Bhattachaya, S.; Chen, G.; **Sheng, R.** Functional Glycopolypeptides: Synthesis and Biomedical Applications . *Adv. Polym. Technol.* **2020**, *2020*, 6052078-. (IF: **1.539**) Q2 (Chemical Engineering)
- **30. Algarra, M.**; Soto, J. Insights into the Thermal and Photochemical Reaction Mechanisms of Azidoacetonitrile. Spectroscopic and MS-CASPT2 Calculations . *ChemPhysChem* **2020**, *21*, 1126-1133. (IF: **3.077**) Q1 (Physical and Theoretical Chemistry)
- **31. Alves, V. L. G.**; **Gonçalves, J. L. J.**; **J. Aguiar**; **Teixeira, H. M.**; **Câmara, J. d. S.** The synthetic cannabinoids phenomenon: from structure to toxicological properties. A review . *Crit. Rev. Toxicol.* **2020**, 1-24. (IF: **4.257**) Q1 (Toxicology)
- **32.** Wang, J.; Lu, S.; **Sheng, R.**; Fan, J.; Wu, W.; Guo, R. Structure-activity Relationships of Natural and Synthetic Indole-derived Scaffolds as α-Glucosidase Inhibitors: A Mini-review . *Mini reviews in medicinal chemistry* **2020**, *20*, 1-. (IF: **2.733**) Q2 (Drug Discovery)
- **33.** Ureta, M. M.; **Martins, G. N. G.**; **Figueira, O.**; **Pires, P. F. D. L.**; **Castilho, P. C. M. F.**; Gomez-Zavaglia, A. Recent advances in β-galactosidase and fructosyltransferase immobilization technology . *Crit. Rev. Food Sci. Nutr.* **2020**, 1-32. (IF: **7.862**) Q1 (Food Science)
- **34. Silva, C. G. S. L.**; **Perestrelo, R. M. d. S.**; Sousa-Ferreira, I.; Capelinha, F.; **Câmara, J. d. S.**; **Petkovic, M.** Lipid biosignature of breast cancer tissues by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry . *Breast Cancer Res. Treat.* **2020**, *182*, 9-19. (IF: **3.831**) Q1 (Oncology)
- **35.** Pinheiro, R. G. R.; Granja, A.; Loureiro, J. A.; Pereira, M. C.; Pinheiro, M.; **Neves, A. R.**; Reis, S. RVG29-Functionalized Lipid Nanoparticles for Quercetin Brain Delivery and Alzheimer's Disease . *Pharm. Res.* **2020**, *37*, 139-. (IF: **3.242**) Q1 (Pharmaceutical Science)
- **36. Silva, Pedro**; **Silva, C. G. S. L.**; **Perestrelo, R. M. d. S.**; Nunes, F. M.; **Câmara, J. d. S.** Application of Quality-by-Design Approach in the Analytical Method Development for Quantification of Sugars in Sugarcane Honey by Reversed-Phase Liquid Chromatography . *Food Anal. Meth.* **2020**, *13*, 1634-1649. (IF: **2.667**) Q2 (Food Science)
- **37. Figueira, J. A.**; **Porto-Figueira, P.**; **Pereira, J. A. M.**; **Câmara, J. d. S.** A comprehensive methodology based on NTME/GC-MS data and chemometric tools for lemons discrimination according to geographical origin . *Microchemical Journal* **2020**, *157*, 104933-. (IF: **3.594**) Q2 (Analytical Chemistry)
- **38. Alves, V. L. G.**; **Gonçalves, J. L. J.**; **Figueira, J. A.**; Ornelas, L. P.; **Branco, R. N.**; **Câmara, J. d. S.**; **Pereira, J. A. M.** Beer volatile fingerprinting at different brewing steps . *Food Chem.* **2020**, *326*, 126856-. (IF: **6.306**) Q1 (Food Science)
- **39.** Song, C.; Shen, M.; **Rodrigues, J. M. C.**; **Mignani, S. M.**; Majoral, J.-P.; **Shi, X.** Superstructured poly(amidoamine) dendrimer-based nanoconstructs as platforms for cancer nanomedicine: A concise review . *Coord. Chem. Rev.* **2020**, *421*, 213463-. (IF: **15.367**) Q1 (Inorganic Chemistry)
- **40.** Sousa, A.; Vareda, J.; Pereira, R.; **Silva, C. G. S. L.**; **Câmara, J. d. S.**; **Perestrelo, R. M. d. S.** Geographical differentiation of apple ciders based on volatile fingerprint . *Food Res. Int.* **2020**, *137*, 109550-. (IF: **4.972**) Q1 (Food Science)
- **41.** Zhang, X.; Wu, Yahui; Li, Z.; Wang, W.; Wu, Yaping; Pan, D.; Gu, Z.; **Sheng, R.**; **Tomás, H.** ; Zhang, H.; **Rodrigues, J. M. C.**; Gong, Q.; Luo, K. Glycodendron/pyropheophorbide-a (Ppa)-functionalized hyaluronic acid as a nanosystem for tumor photodynamic therapy . *Carbohydr. Polym.* **2020**, *247*, 116749-. (IF: **7.182**) Q1 (Organic Chemistry)

7TH CQM ANNUAL MEETING

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Events 2019/20

Events 2019


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LAST MINUTE CONFERENCE!
"DEVELOPMENT OF NEW ANALYTICAL PROCEDURES WHICH INVOLVE NANOMATERIALS IN FOOD SAMPLES"
Andrea Gomez-Zavaglia, PhD
Center for Research and Development in Food Cryotechnology (Argentina)
25th JANUARY 2019
15:00 | Conference room 0.57 | Free entrance, no registration required
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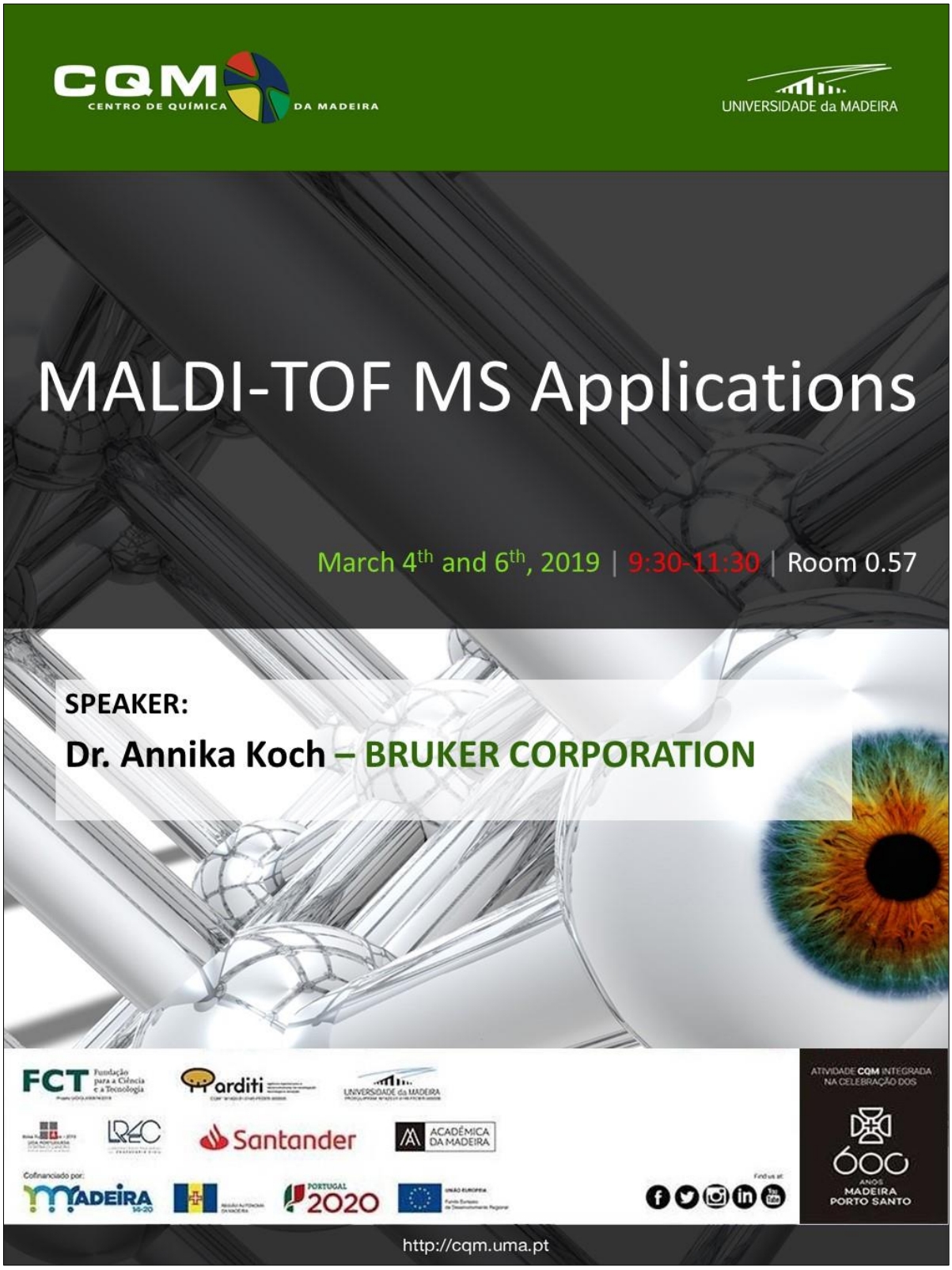
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MALDI-TOF MS Applications
March 4th and 6th, 2019 | 9:30-11:30 | Room 0.57
SPEAKER:
Dr. Annika Koch – BRUKER CORPORATION
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"SCRATCH RESISTANT NON-FOULING SURFACES VIA GRAFTING NON-FOULING POLYMERS ON THE PORE WALLS OF SUPPORTED POROUS OXIDE STRUCTURES"

Mohammed Es-Souni, PhD
Institute for Materials & Surface Technology (IMST), Kiel University of Applied Sciences
Germany

13th MARCH 2019

15:00 | Conference room 0.57
Registration at https://cqm.uma.pt, until 12th March 2019

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Possibilities and Limitations
March 19th | 9h30-10h30 | Room 0.57
SPEAKER:
DR. MARIJANA PETKOVIC - MALDI-TOF Expert
(CQM Senior Member)
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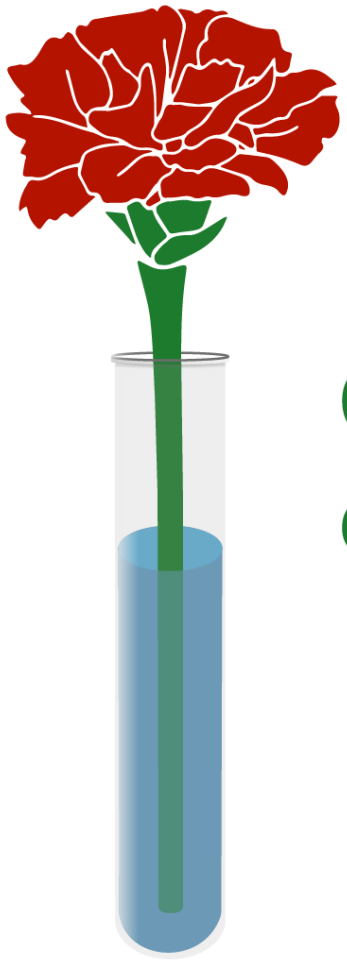

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"EXTREMOPHILIC ENZYMES PRODUCTION, AND USE OF IONIC LIQUIDS AS SEPARATING AGENTS"
Dr. María Asunción Longo
Department of Chemical Engineering, University of Vigo, Spain
16:00
"NUTRACEUTICAL COMPOUNDS PRESENTS IN THE LEAVES OF COFFEA"
Dr. Maria Teresa Salles Trevisan
Federal University of Ceará, Brazil
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"SUSTAINABLE VALORIZATION OF RESIDUES FROM THE FOOD INDUSTRY: OBTAINING BIOACTIVE PEPTIDES"

Maria Luisa Marina, PhD
University of Alcalá (Spain)

03rd JULY 2019

15:00 | Amphitheatre 05 | Free entrance, no registration required

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10h00 - Receção e introdução (ILC)
10h15 - Apresentação da linha de Cromatografia PURE (Daniel Rocha, ILC)
11h00 - Coffee Break
11h20 - Sessão Prática com o sistema FLASH e Preparativo PURE C-850
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04 MARÇO'2020 09H45

Escola Básica 2/3 Ciclos Dr. Horácio Bento de Gouveia

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2020
21-22
September
AUDITÓRIO DO COLÉGIO DOS JESUÍTAS
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PARTNERS AND FINANCIAL SUPPORT
FCT Fundação para a Ciência e a Tecnologia
BASE FUND - UIDB/00674/2020
REPÚBLICA PORTUGUESA
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MADEIRA 14-20
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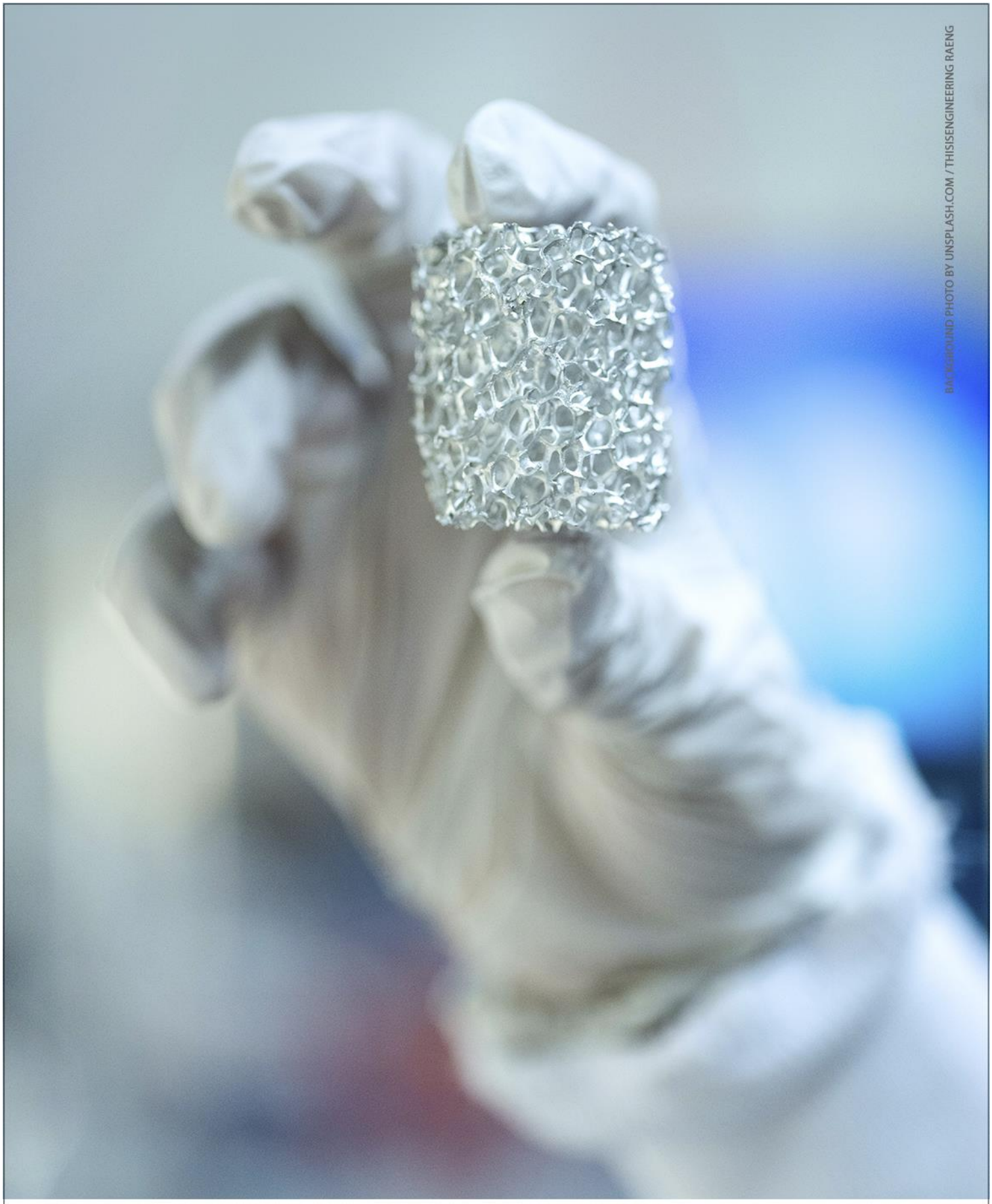

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PARTNERS AND FINANCIAL SUPPORT

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CQM*: M1420-01-0145-FEDER-000005

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