

**PTIM** '23  
POLLUTANT TOXIC IONS & MOLECULES

5<sup>th</sup> International Caparica  
Conference on Pollutant Toxic Ions  
& Molecules 2023

6<sup>th</sup> – 9<sup>th</sup> November 2023  
Caparica – Portugal

# BOOK OF ABSTRACTS

5<sup>th</sup> International Caparica Conference on  
Pollutant Toxic Ions and Molecules 2023

**Hotel TRYP Lisboa Caparica Mar**  
**Caparica | Portugal**



**PROTEOMASS**

SCIENTIFIC SOCIETY

## **PTIM 2023**

5<sup>th</sup> International Caparica Conference on Pollutant Toxic Ions and Molecules 2023

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Caparica – Portugal, 2023

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## **WELCOME 5<sup>th</sup> PTIM 2023**

### **5<sup>th</sup> International Caparica Conference on Pollutant Toxic Ions and Molecules 2023**

Warm Greetings to the Esteemed Participants of the 5th International Caparica Conference on Pollutant Toxic Ions and Molecules!

We are delighted to welcome you to the charming coastal town of Costa de Caparica, Portugal, which hosted this enlightening conference from November 6th to 9th, 2023. This pivotal event united experts, researchers, and practitioners from 28 nations, fostering a vibrant exchange of innovative ideas and findings in environmental science.

In a time characterized by unparalleled industrial and urban growth, pollution and its extensive repercussions have emerged as a global dilemma. Pollutant toxic ions and molecules, originating from diverse sources like

## WELCOME

industrial activities, agriculture, and urban runoff, pose a significant threat to ecosystems, human health, and our planet. A deep understanding of these pollutants, their behaviors, and impacts across various environments is vital for crafting effective mitigation strategies and policy actions.

The conference carved out a distinctive platform for multidisciplinary dialogues, enabling specialists from varied fields such as chemistry, environmental science, toxicology, public health, policy, and engineering to disseminate their most recent research outcomes, insights, and technological advancements. The objective was to encourage collaboration, bridging theoretical and practical divides, and facilitating the development of sustainable solutions to challenges presented by pollutant toxic ions and molecules.

The scenic village of Caparica, with its breathtaking coastline, served as a motivational setting for this scholarly exchange. Enriched by Lisbon's cultural heritage, exquisite local cuisine, and stunning vistas of the Atlantic Ocean, Caparica provided a vibrant atmosphere for participants to engage in profound discussions, forge valuable networks, and explore new research avenues.

This volume encompasses the works presented at the conference, covering a broad array of topics related to pollutant toxic ions and molecules. The papers herein demonstrate pioneering research methodologies, innovative technologies, and fresh insights into pollutants' sources, fate, transport, and impact. We aspire for these proceedings to serve as a precious resource for scholars and researchers and to further the global discourse on environmental sustainability.

Our sincere thanks go to all authors, presenters, attendees, sponsors, and organizers who played a part in making this conference a triumph. Their commitment and zeal have marked this event as a significant landmark in the pursuit of a cleaner and healthier planet.

The PTIM conference series has firmly positioned itself as a leading international scientific forum, covering environmental, chemical, health, and well-being sciences. Previous editions in 2015, 2017, 2019, and 2021 explored topics like emerging toxic contaminants, broader pollution issues, detection and protection trends, and health implications. The 2023 edition symbolizes a rekindling of connections, promoting collaboration to protect the environment and health amidst the dual challenges of climate change and global pollution post-pandemic.

In 2023, our plenary speakers include eminent figures like Professors Irene MC Lo (Hong Kong), Tamara García Barrera (Spain), Damiá Barceló (Spain), Joanna Burger (USA), Jorg Rinklebe (Germany), Jay Gran (USA), and Sergey Shabala (Australia). Moreover, a lineup of outstanding keynote and KPRK speakers including José Luis Gomez Ariza (Spain), Franz Jirsa (Austria), Jakub Zdarta (Poland), Rut Fernandez Torres (Spain), Maria Ramos Payan (Spain), Michael Gochfeld (USA), Artur Badyda (Poland), Philishwa Nomngongo (South Africa), Jurgen Gailer (Canada), Luiza Campos (UK), and Elisabete Oliveira (Portugal). With 150 participants from 28 countries presenting 7 Plenary talks, 14 Advanced Keynotes, 40 oral presentations, 30 posters, and 27 shotgun presentations (both oral and poster), elevates the conference to a paramount environmental protection and health discussion event.

On behalf of the BIOSCOPE Research Group, the PROTEOMASS Scientific Society, The LAQV-REQUIMTE Laboratory, the FCT-NOVA, NOVA University Lisbon, we are thrilled to welcome you to the 5th edition of the International Caparica Conference on Pollutant Ions and Molecules, PTIM2023. Your attendance and participation symbolize a steadfast dedication to preserving our environment and ensuring global health.

**Carlos Lodeiro, MSc PhD FRSC**

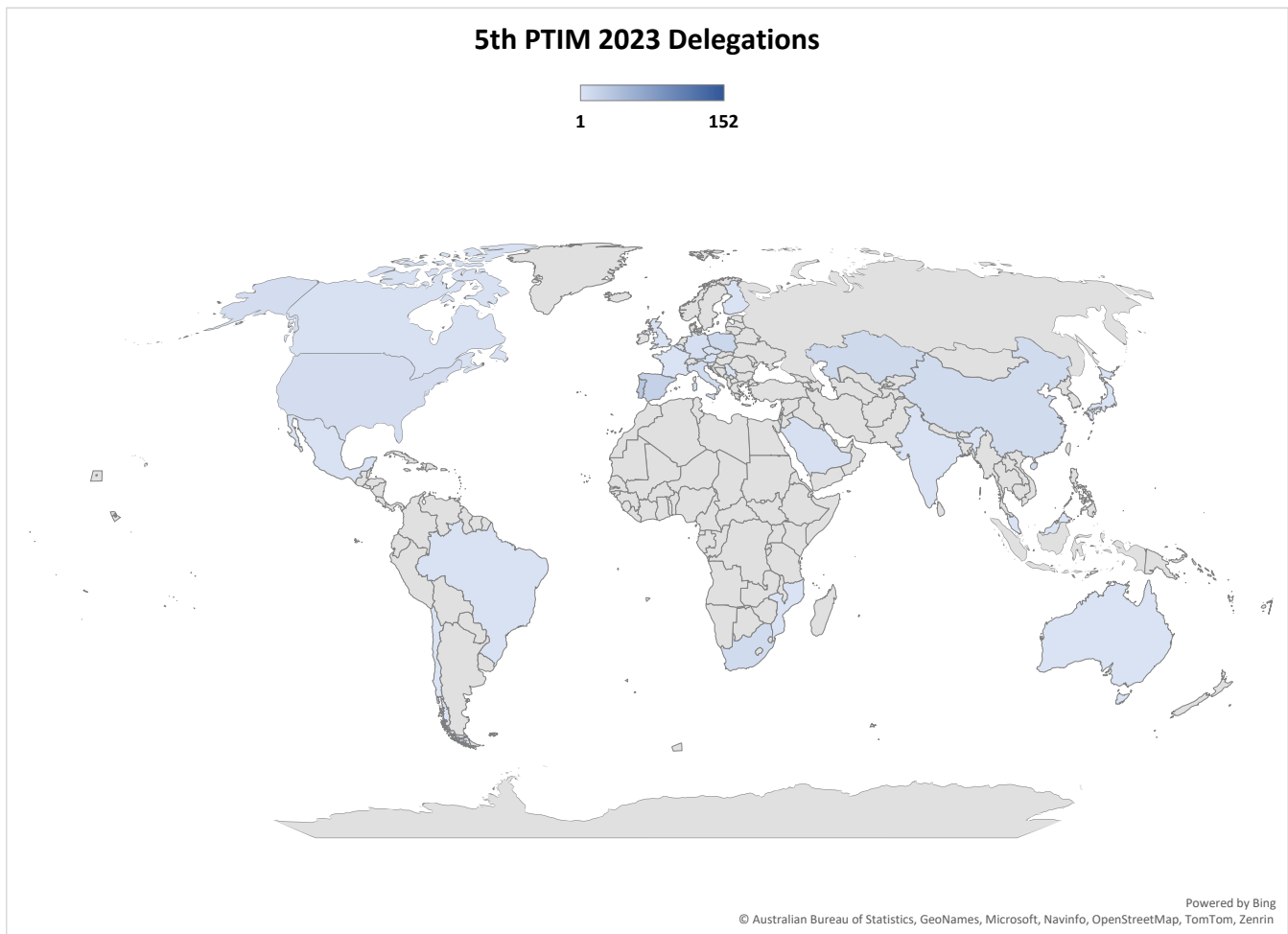
**José Luis Capelo-Martínez, MSc PhD FRSC**

Hugo M. Santos, MSc PhD PhD

Elisabete Oliveira, MSc PhD PhD

Chairs

5<sup>th</sup> PTIM 2023 - Participants' Demographics



**Figure 1** - Participants in the 5<sup>th</sup> PTIM 2023 Conference by country: Australia (1), Austria (3), Belgium (1), Brazil (2), Canada (3), Chile (1), China (9), Czech Republic (2), Finland (1), France (1), Germany (5), India (2), Israel (3), Italy (8), Japan (1); Kazakhstan (12), Malaysia (1), Mexico (2), Mozambique (1), Poland (14), Portugal (30), Saudi Arabia (4), Serbia (3), Slovenia (1), Singapore (2), South Africa (10), Spain (20), United Kingdom (2), United States of America (7)



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## ***COMMITTEES***



## CONFERENCE CHAIRS

### José Luis Capelo Martínez



Head of the Bio-analytics & Proteomics Laboratory  
BIOSCOPE Research Group & (Bio)Chemistry and OMICS Group,  
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Dr. J. L. Capelo, a distinguished researcher and Associate Professor in the Chemistry Department (Biochemistry) at FCT NOVA, has carved a notable path in Analytical Proteomics. Earning his PhD from the University of Vigo (Spain) in 2002, he embarked on a post-doctoral position at IST-UL in Lisbon (2002-2005), followed by a research position at REQUIMTE (FCT-NOVA, 2005-2009). His journey then took him back to the University of Vigo as a Principal Investigator (2009-2012) before being appointed as an Assistant Professor at FCT-NOVA in 2012. A Fellow of the Royal Society of Chemistry and a member of the Portuguese Chemistry Society, Dr. Capelo achieved habilitation in Analytical Proteomics in Portugal at FCT-NOVA in 2017, subsequently becoming an Associate Professor. He co-leads the BIOSCOPE research group and holds the position of Chairman at the PROTEOMASS Scientific Society, alongside being the Founder and co-CEO of the Chemicals start-up Nan@rts.

Dr. Capelo's research spans various topics, including the quantification of metal and metal species in environmental and food samples, developing methods for speedy protein identification using mass spectrometry-based workflows, bacterial identification via mass spectrometry, and exploring applications of nanoparticles in nano-proteomics and nanomedicine, among others. Having mentored 12 PhDs with an additional 4 in progress, Dr. Capelo continues contributing significantly to the field, guiding the next generation of researchers and exploring innovative avenues in environmental science and proteomics.

## COMMITTEES

### Carlos Lodeiro Y Espiño



Head of the Chemistry & Nano-synthesis Laboratory  
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Dr. C. Lodeiro graduated in Chemistry in 1995, and received his PhD in chemistry in 1999 from the University of Santiago de Compostela, Spain. In 1999 he moved to the NOVA University Lisbon (NOVA), Portugal as a European Marie Curie postdoctoral researcher in a project concerning molecular devices and machines, and in 2004 he became a fellow researcher and invited assistant lecturer at the REQUIMTE-CQFB, Chemistry Department (NOVA). In 2008 Dr. Lodeiro got the habilitation in Chemistry in Spain, and a year later in 2009 he moved to the University of Vigo, Faculty of Sciences of Ourense (FCOU), Spain as IPP (Isidro Parga Pondal) researcher-lecturer. In 2012 became Assistant Professor at the Chemistry Department UCIBIO-REQUIMTE Laboratory in the NOVA School of Science and Technology, FCT-NOVA. Dr. Lodeiro is a Fellow of the Royal Society of Chemistry since 2014 and member of the Portuguese Chemistry Society since 2002, and the American Chemical Society since 2016. In 2017 got the habilitation in Inorganic Analytical Chemistry in Portugal at the FCT NO and became Associate Professor in the Chemistry Department FCT-UNL. Presently he co-leads the BIOSCOPE research group ([www.bioscopegroup.org](http://www.bioscopegroup.org)), he is CEO of the PROTEOMASS Scientific Society, and Founder co-CEO of the Chemical start-up Nan@rts. His research interest comprises (i) physical-organic and physical-inorganic chemistry of dyes and chemosensors, (ii) synthesis of Functionalized Nanoparticles, Nanocomposites and Nanomaterials (iii) applications of nanomaterials in environmental research, (iv) application of nanomaterials in bio-medical research, (v) supramolecular analytical proteomics, and (vi) Onco and Nanoproteomics. C. Lodeiro has mentored 12 PhDs plus 3 in course.

## Hugo Miguel Santos



Head of the Laboratory for Biological Mass Spectrometry & Functional - Associations of Post-Translational Modifications - Head of the Laboratory for Biological Mass Spectrometry - Isabel Moura - BIOSCOPE Research Group & (Bio)Chemistry and OMICS Group, LAQV-REQUIMTE, Department of Chemistry - NOVA School of Science and Technology, NOVA University Lisbon (Caparica, Portugal) - Chief Proteomics Technology Officer PROTEOMASS Scientific Society  
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HM Santos began his career in Proteomics in 2007, embarking on a joint PhD program in Biochemistry at NOVA University Lisbon (Portugal) and the Turku Centre for Biotechnology (Finland) working with state-of-the-art MS instrumentation for biomedical research. H.M. Santos took up a post-doc at the University of Vigo (2010-12 to 2011-03) followed by a move to the Institute of Biomedicine and Biotechnology (Barcelona, Spain, 2011-04 to 2012-03) to advance biomedical applications of mass spectrometry and translational research. In 2011 H.M. Santos moved to FCT NOVA to continue his research in Biological Mass Spectrometry. Currently, he is Assistant Researcher at LAQV-REQUIMTE FCT NOVA (Portugal). H.M. Santos is Member of the Royal Society of Chemistry. His scientific interests are focused on (i) Identification of molecules involved in complex biological processes, characterize their structure and monitor how their abundance may change during these processes, in order to gain insights into the underlying molecular mechanisms; (ii) nano-proteomics and nano-medicine; (iii) application of chemosensor to the detection/quantification of metals; (iv) Mass spectrometry analysis of organic molecules, metal complexes and supramolecular systems. To date, he has mentored 6 PhDs.

### Elisabete Oliveira



Head of the Laboratory for Mesoporous Silica Materials  
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Dr. E. Oliveira graduated, in 2006, in Applied Chemistry from FCT- Nova University Lisbon, Portugal, in 2007 obtained a master's in biotechnology and completed a PhD degree in Biotechnology in 2010, at the same University. In 2013, she obtained a second PhD degree in "Food Science and Technology" by the Science Faculty of Ourense Campus at the University of Vigo, Spain. Currently, she is Assistant Researcher at LAQV-REQUIMTE FCT NOVA (Portugal). In 2008, E. Oliveira received the prize in Creativity and Quality in Research Activity in sensors area, attributed by Foundation Calouste Gulbenkian, Portugal and in 2016 she was awarded with the Prize For Women in Science, "Medalhas de Honra L'Oréal Portugal para as Mulheres na Ciência" in the field of health Sciences. Her scientific interests are focused in (i) synthesis of new bio-inspired emissive ligands as fluorescence chemosensors, (ii) supramolecular chemistry (Photophysics and photochemistry), (iii) applications in vitro (solution and solid studies) and in vivo (cell imaging studies); (iv) synthesis of new emissive nanomaterials, as Quantum Dots and Mesoporous Silica nanoparticles for dual drug delivery and biomarker discovery in biological samples, and (v) Antibacterial studies of cargo-delivery mesoporous nanoparticles. To date, she has mentored 1 PhD plus 3 in course.

## **SCIENTIFIC COMMITTEE**

### **Adrián Fernández-Lodeiro | MSc | PhD | MRSC**

University of Cyprus School of Engineering, Department of Electrical and Computer Engineering (Cyprus)

### **Carlos Lodeiro Espiño | MSc | PhD | FRSC**

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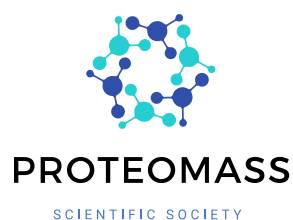
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## P.8 Engineered Biochar Made from Waste Plum Stones as Efficient Sorbent in Phosphate Removal.

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The concerns over the environmental and economic issues of the phosphates as eutrophication agents are continuously rising, due to their toxic effects on the whole environment. The greatest risk arises from entering phosphates into water streams as the runoff from agricultural lands and those from sewage water. Among the conventional methods used for phosphate removal, adsorption technology appeared as the most promising one, due to its simplicity and economical feasibility. Another advantage of this technique is the possibility of sorbent regeneration with low amounts of by-products, and possible reuse of regenerated sorbate in different applications, including agriculture. Amongst many sorbents widely used, modified activated carbon (AC) is mostly used, but the application of modified AC raises costs of AC production/application. In the sense of this, the search for cheaper sorbents with higher phosphate removal capacity is still needed. Biochar (BC) is a cost-effective and environmental friendly stable solid material rich in carbon, resistant to decomposition and mineralization [1]. Although BC and AC are made from similar raw materials, BC is usually produced at lower temperatures, resulting in a price of BC that is app. 1/6 of the price of the commercial AC [2]. In the last decade, BC is receiving great attention as a promising sorbent for different pollutants from water streams, but the use of BC also supports the reduction of greenhouse gases and its application into soils enhance the soil fertility. Many recent studies with unmodified BCs [3] have shown lower phosphate removal ability, indicating negative surface charge as one of the factors influencing lower removal of negatively charged ions over a wide pH range. In order to increase BCs sorption capacity toward phosphates, the introduction of some cationic species is often required. In this paper, synthesis of MgO-biochar from waste lignocellulosic biomass was applied, in order to create highly porous nanocomposite material with efficient phosphate removal. For this purpose, feedstock used to make the MgO-biochar nanocomposites were plum stones (PmS) obtained from the local factory, where they have been disposed as a waste. After receiving, feedstock was air dried and milled into 0.1-0.5 mm particles. MgCl<sub>2</sub>·6H<sub>2</sub>O was used to prepare a solution to pre-treat the PmS feedstock according to the procedure described in [4]. After immersing procedure, the oven dried mixture was heated at 10 °C/min up to 500 °C under Ar flow for 1,5 h. For the purpose of sorbent characterisation, pH<sub>pzc</sub>, XRD, TG-DTG and FTIR analysis were performed. The existence of Mg nanoparticles shifts the pH<sub>pzc</sub> from 6.7 to highly alkaline value of 10.7 which facilitates the electrostatic interactions between the negatively charged PO<sub>4</sub><sup>3-</sup> ions and PmS-M-B. The diffraction peaks identified as MgO revealed that MgO particles were highly crystalline, and uniformly deposited across the entire PmS-M-B surface. TGA analyses revealed four stage degradation, where the peaks for the PmS-M-B shifted to the higher temperatures compared to the unmodified biochar (PmS-B) and higher residual mass after final combustion stage. FTIR spectra have showed most band differences in the 1800–600 cm<sup>-1</sup> range. The characterised MgO-biochar nanocomposite produced from pyrolysis (PmS-M-B) was further used in sorption experiments. A stock phosphate solution was prepared using KH<sub>2</sub>PO<sub>4</sub> and diluted to the required concentrations. The adsorption isotherm of phosphate on the PmS-M-B was determined using the batch sorption technique by mixing 0.1 g of the biochar sample with 50 mL of phosphate solutions of different concentrations ranging from 10 to 500 mg/L. The reaction vessels were shaken (150 rpm, 25 °C) and after the desired contact times (from 5 min to 24 h), the samples were filtered, phosphate concentrations in the liquid phase samples were determined using MD 610 colorimeter (Lovibond, Germany), and the amount of PO<sub>4</sub><sup>3-</sup> adsorbed onto PmS-M-B was calculated. Data obtained through the isothermal experiments were fitted using three commonly applied isotherms: Langmuir, Freundlich and Sips. Isotherm equilibrium modelling revealed that the Sips isotherm provided the best model fit with maximum sorption capacity of 181.46 mg/g. This sorption capacity is much higher than the most of the others reported in literature [5, 6]. A possible sorption mechanism of PO<sub>4</sub><sup>3-</sup> removal might be assigned to electrostatic attraction and hydrogen bonding. Obtained results demonstrated that engineered MgO-biochar derived from waste PmS can be used as a promising green material for removing phosphates from contaminated waters, providing opportunities in developing low-cost and highly efficient material to resolve eutrophication issue. In the same time, environmental benefits might be multiple: decreasing environmental hazards by reducing waste landfills, and also using exhausted sorbate in soil remediation and as a slow release fertilizer, confirming advantages of the biochars amongst the other available adsorbents.

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