



ChIR Symposium 2023

 **3RD - 4TH JULY**

 **University of Algarve, Faro**

Book of Abstracts

Welcome to the ChIR Symposium, 2023!

Celebrating a decade of the ChIR Erasmus Mundus Project

Welcome to the ChIR Symposium celebrating 10 years of an extraordinary project, the Erasmus Mundus MSc in Chemical Innovation and Regulation - ChIR! We are thrilled to commemorate the journey of the ChIR project over the past decade, and we invite you to join us in this momentous occasion.

For a decade, the ChIR has united brilliant minds from diverse disciplines, cultures and backgrounds, with the common aim of studying and researching how to achieve safety and sustainability in chemical substances and chemical industry activities.

This year the symposium aims to commemorate the success and impact of the program while continuing to provide an opportunity for alumni, researchers, current students, and industry professionals to connect, exchange ideas, and explore new horizons in chemical innovation and regulation.

Similar to last year's, the event will be streamed online allowing those who cannot travel to Faro the opportunity to follow it remotely.

Join us at the Symposium and let us embark on this inspiring voyage of knowledge, discovery, and progress!

ChIR Symposium Sponsors



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ChIR Symposium Programme Timetable

<http://emmcchir.org/symposium2023/>

Monday, July 3

8:30	Registrations		
9:00	Opening session		
Session 1 Environmental Sustainability			
<i>Chairperson: Emilio Tagliavini</i>			
9:15	Plenary 1	<i>Maria de Lurdes Cristiano</i>	Artemisinin and related endoperoxides: from the treatment of Malaria to applications in Aquaculture
10:15	Coffee break		
10:30	TP1	Erika Martinelli	Supramolecular tools for the molecular recognition of environmental contaminants.
10:45	TP1	Adriana Gonzalez Alcivar	Biodegradation of conventional and biodegradable microplastics
11:00	TP3	Charles Kofi Ayi	Performance of Advanced Oxidation Processes for micropollutant removal contained in urban wastewater
11:15	<i>Discussion</i>		
11:30	TP4	Reyhan Ammar	Emerging pollutants removal by advanced oxidation processes: A case of study with nanoplastics
11:45	TP5	Yusuf Ibrahim	UV-assisted activation of different oxidants for wastewater remediation: feasibility and comparative study
12:00	TP6	Juan Francisco Chajón Villatoro	Study of 2D materials for sustainable conversion of CO ₂ through catalysed processes
12:15	<i>Discussion</i>		
12:30	Lunch		
Session 2 Chemical Industry			
<i>Chairperson: Alessandra Tolomelli</i>			
14:30	Keynote 1	<i>Askar Nurassilov</i>	Global chemical registration as a pass to the international market
15:15	TP8	Gisela Obregón Gutiérrez	Solvent assessment and selection in terms of sustainability, performance, and cost.
15:30	TP9	Marcelo Martínez	Greening active pharmaceutical ingredients synthesis: use of alternative biogenic solvents in solid phase peptide synthesis
15:45	<i>Discussion</i>		
16:00	TP10	Aladdin Mardanov	Mechanosynthesis of fluorinated active pharmaceutical ingredients
16:15	TP11	Majid Esmaeili	Designing a long-lasting corrosion inhibitor for an innovative solution
16:30	TP12	Ariana Gabriela Neyra Pérez	Metal organic framework nanosheets of metal-catecholate for chemical sensing.
16:45	<i>Discussion</i>		
17:00	Coffee break		
	(Poster Session)		

Tuesday, July 4

Session 3 Regulation

Chairperson: Daniel Sainz

9:30	Plenary 2	Montserrat Filella	The journey towards ending plastic pollution
10:30	Coffee break		
10:45	TP13	Carla Thaís	Comparison of risk and sustainability of different PLA reinforcements for production of filaments in 3D printing
11:00	TP14	Mariana Martínez	Comparative analysis of chemical regulations in Mexico, US and EU
11:15	<i>Discussion</i>		
11:30	Keynote 2	Ester Carregal	The Future of chemicals risk assessment at the OECD

Session 4 Chemistry from Nature

Chairperson: Isabel Cavaco

12:00	TP15	Segismundo García Valverde	Isolation and identification of bioactive compounds from microalgae
12:15	TP16	Hector Romero	Exploring the medicinal halophytes Limonium algarvense and Polygonum maritimum as sources of cosmetic ingredients
12:30	<i>Discussion</i>		
12:45	Lunch		

Session 5 Health and Food

Chairperson: Santiago Esplugas

14:45	Keynote 3	Ana Vallejo	Life after ChiR: Lessons learned at ECHA and agricultural industry
15:15	TP17	Negussie Darota	Inorganic Nanocomposites as dual therapeutic agents
15:30	TP18	Fajar R. Putera	Computational modelling of taste receptors.
15:45	TP19	Letícia Anjinho de Barros	Development of nanoemulsification technologies with application in food: Application to the preservation of fresh food and the incorporation
16:00	<i>Discussion</i>		
16:30	Coffee break		
16:30	(Poster Session)		
17:15	Closing session		

Plenary Abstracts

Artemisinin and related endoperoxides: from the treatment of Malaria to applications in Aquaculture

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Organic peroxides are found in various natural products, as biologically active compounds, and take part in chemical reactions, as intermediates. The interest in cyclic organic peroxides is mainly due to the 1,2,4-trioxane pharmacophoric moiety of artemisinin (ART), since this natural product and some of its semi-synthetic derivatives integrate the arsenal of frontline antimalarial drugs.

Meanwhile, the rise and spread of *Plasmodium falciparum* resistance to artemisinin-based combination therapy, in Southeast Asia, stimulated the search for novel plasmodial “fast killers” and synthetic endoperoxide-derived compounds have been shown to offer alternative solutions to artemisinin and its derivatives (ARTs). Selected synthetic 1,2,4-trioxanes, 1,2,4-trioxolanes and 1,2,4,5-tetraoxanes proved particularly promising in this context, exhibiting anti-malarial activity similar or higher than ARTs, including against multi-resistant *P. falciparum* strains, as is the case for antimalarial candidates OZ439 and E209. In parallel, synthetic routes for those compound classes have been developed and perfected, enabling the preparation of a chemically diverse range of analogues for selection of leads, optimization, and development into anti-malarial drugs or drug candidates.

Although remaining under debate, the mechanism of bioactivation and action of endoperoxide-based drugs has been discussed thoroughly. Bioactivation is thought to require Fe(II)-induced reductive cleavage of the peroxide bond, forming oxygen-centered radicals that subsequently rearrange to generate carbon-centered radicals, these acting through the alkylation of parasites’ biological targets.

Given the alkylating potential and multitarget nature of endoperoxides action, synthetic five- and six-membered 1,2,4-trioxolanes, 1,2,4-trioxanes and 1,2,4,5-tetraoxanes were scrutinized for their applicability in the treatment of other infections, namely those due to other Protozoa parasites, and of cancer. To this end, a diverse range of novel endoperoxides came to light. Some were designed within the “molecular hybridization” concept, whereby an endoperoxide moiety is linked to other pharmacophores, leading to novel hybrid molecules. These more complex structures were meant to afford pharmacological benefits when compared to the parent drugs,

such as better efficacy, improved safety, cost-effectiveness, and less vulnerability to resistance selection, in view of their application to the treatment of human diseases.

On the other hand, the knowledge on the structure, reactivity and properties of endoperoxides, allied to the availability of amenable synthetic routes to their preparation from cheap starting materials, stimulated research on use for the treatment of protozoan infections that affect marine species, namely in the aquaculture sector, thereby preventing heavy economic losses and social constraints.

The present lecture is dedicated to the ChIR students and Alumni. I will approach the issues mentioned above, integrating some scientific contributions from present and past researchers of the OrgMedChem laboratory of CCMar and of FCT/UAlg.

Acknowledgements: We thank the Fundação para a Ciência e a Tecnologia for Grants SFRH/BD/130407/2017 (PSMA) and SFRH/BD/08242/2020 (ICCC), and projects UIDB/04326/2020, UIDP/04326/2020 and LA/P/0101/2020 (CCMAR); CRESC Algarve 2020 and COMPETE 2020 are also acknowledged, for project EMBRC.PT ALG-01-0145-FEDER-022121.

The journey towards ending plastic pollution

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Plastics have become ubiquitous in our modern life because of their light weight, low cost and versatility. As a result, global plastic production has increased exponentially since the 1950s, reaching some 460 million tons in 2019. Continued growth in annual global primary plastic production is currently on track to possibly reach 1.1 billion tons in 2050. Meanwhile, the world has seen a huge increase in plastic waste in the environment and many associated adverse impacts on ecosystems. Concerned about the impact of plastic pollution, the United Nations Environment Assembly (UNEA) adopted a resolution in March 2023, calling for the development of an international legally binding instrument by the end of 2024, to be adopted at the first Conference of Parties mid-2025. The UNEA resolution was the starting point of an intensive negotiation process under the leadership of the Intergovernmental Negotiating Committee (INC). The treaty is to be based on a comprehensive approach addressing the entire life cycle of plastics. This includes all plastic components. The bulk component of plastics is a polymer made from repeating chemical monomer units, up to 99% sourced from fossil raw materials but other chemicals are added as processing aids (lubricants) or as additives (plasticizers, flame retardants, heat and light stabilizers or pigments). According to recent data, more than 30 million tons of processing aids and plastic additives are used each year. Of the 13,000 chemical substances associated with plastics, 7,000 have been screened for their hazardous properties, of which more than 3,200 have one or more hazardous properties of concern, i.e., the potential to exert significant impacts on human health and the environment.

This lecture will address different aspects of the uses, composition, and pollution of plastics with the aim of understanding the background and the treaty process. The need for an effective global plastics treaty, based on sound, evidence-based decisions, will be emphasized.

Keynotes Abstracts

Global chemical registration as a pass to the international market

Askar Nurassilov

Global Chemical Control Legislation Professional



In recent decades, there has been an intense development of various chemical management systems around the globe. While some countries have built on the existing mechanisms, others followed a path paved by EU REACH or created their own unique way of regulating chemicals. Furthermore, the trend continues with fast-paced emerging regulations in LATAM, APAC and other regions. Regardless of the overall approach chosen by the countries, the global chemical control regulation is undoubtedly paramount for the safe use of chemicals, human health safety and environmental protection.

In any established chemical management system, a registration aspect represents a pass for any business to access the global market. Despite the general intention to harmonise regulations around the globe, the differences still prevail and lead to significant challenges and costs for the companies when attempting to step into the international playground. Therefore, it is crucial to understand the differences, find harmonies in order to build a robust global registration strategy. This presentation aims at providing a global perspective on chemical registrations which should serve as a basis line for an early-stage global chemical regulations professional.

The future of chemicals risk assessment at the OECD

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At the event to commemorate the 50-year anniversary of the OECD Chemicals Programme held in February 2022, the OECD took the opportunity to review some of the Programme's accomplishment of the last decade and to consider the future of risk assessment, including some of the innovative biotechnology tools, advances in molecular understanding of toxicity, shifting regulatory requirements, and the need for chemical safety information for an increasing number of chemicals entering commerce.

The Future of Risk Assessment is focused on new approach methods (NAMs) for evaluating chemical hazards, accordant with the initiatives promoted by countries and regulatory authorities to improve acceptance and use of NAMs in a regulatory context. While the increase in use of NAMs is commendable, lack of international harmonization in acceptance and application of these approaches can lead to the erosion of the benefits of Mutual Acceptance of Data (MAD) [1] and may lead to loss of efficiencies and increases in costs for industry and governments.

The OECD works on standards, tools, guidance, and approaches to build confidence in NAMs. Notable examples are the Integrated Approaches to Testing and Assessment (IATA) Case Studies project [2], and the Adverse Outcome Pathways project [3]. Considerable progress in the standardisation of NAMs is also being achieved through OECD's Test Guidelines Programme. Recent advances include the finalisation of Test Guidelines for Defined Approaches for human dermal sensitisation [4] and eye irritation [5].

These OECD activities are informed by various national and international initiatives to implement NAMs in chemical safety assessments to increase the throughput, decrease the cost of safety testing, develop methods that are more human relevant, and do so with reduced or no need for the use of animals. In the next decades, the OECD will continue to play an important role in harmonising the review, documentation, and application of NAMs for global chemical assessment.

References: [1] <https://www.oecd.org/chemicalsafety/testing/mutualacceptanceofdatamad.htm>
[2] <https://www.oecd.org/chemicalsafety/risk-assessment/iata/>
[3] <https://www.oecd.org/chemicalsafety/testing/adverse-outcome-pathways-molecular-screening-and-toxicogenomics.htm>
[4] https://www.oecd-ilibrary.org/environment/guideline-no-497-defined-approaches-on-skin-sensitisation_b92879a4-en
[5] https://www.oecd-ilibrary.org/environment/test-no-467-defined-approaches-for-serious-eye-damage-and-eye-irritation_28fe2841-en

Life after ChiR: lessons learned at ECHA and agricultural industry

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European Chemicals regulation is an intricate, comprehensive and yet connected legislative framework. The implementation of a complex and interdependent network of regulations for chemical substances, including industrial chemicals, plant protection products, biocides, or chemicals in food and feed is challenging [1]. However, it is one of the most comprehensive and protective regulatory frameworks for chemicals [2]. European Commission, member state competent authorities and scientific experts work on this difficult task to make sure the pieces of the puzzle fit together with the goal of protecting human health and environment.

I had the opportunity to experience two sides of the process after graduating ChiR. The first one when I joined ECHA (European Chemical Agency). Our day to day involved engaging with internal and external stakeholders, providing support from the regulatory perspective, IT submission tools (IUCLID, REACH-IT) as well as ECHA's dissemination platform. It was during this time that I learned the most about REACH [3] and CLP [4] regulations. I also experienced the challenges EU agencies face on making sure the companies comply with the regulatory obligations at ECHA.

While working at the industry of agriculture I have learned about plant protection regulation (EC 1107/2009) [5], EU fertilizer regulation (EC 1009/2019) [6], EU organic input regulation (EU 2018/848) [7]. Pesticide legislation being the most stringent. Although pesticides represent the backbone of the agri-food sector there are concerns related to their adverse effects on human health and environment [8]. Kimatec develops products that aim for sustainable agriculture with a good investment in R&D. However, registering these innovative products is a daily challenge as the current legislation is mainly focused on conventional agrochemicals. There is still a lot to learn on chemical regulations but having this valuable working experience brings me a step closer.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD. ECHA and Kimatec working colleagues.

References: [1] Millstone, E. Clausing, P. Reasons for reinforcing the regulation of chemicals in Europe; *European Journal of Risk regulation* **2023** vol 14, 78-92. [2] European Commission, Chemicals Strategy for Sustainability Towards a Toxic-Free Environment, COM 667. **2020** [3] Regulation (EC) No 1907/2006 on the Registration, Evaluation, Authorisation and Restriction of Chemicals. OJ L 396, 30.12.2006 [4] Regulation (EC)

No 1272/2008 on the Classification, Labelling and Packaging of Substances and Mixtures. OJ L 353, 31.12.2008
[5] Lykogianni, M. et al. Do pesticides promote or hinder sustainability in agriculture? The challenge of sustainable use of pesticides in modern agriculture, *Science of the total environment*, **2021** vol 795 [6] Regulation (EC) No 1107/2009 concerning the placing of plant protection products on the market and repealing Council Directives 79/117/EEC and 91/414/EEC [7] Regulation (EU) 2019/1009 laying down rules on the making available on the market of EU fertilising products and amending Regulations (EC) No 1069/2009 and (EC) No 1107/2009 and repealing Regulation (EC) No 2003/2003 (EC) [8] Regulation (EU) 2018/848 on organic production and labelling of organic products and repealing Council Regulation (EC) No 834/2007.

**Research Theses Presentations
Abstracts
(Oral and Poster)**

Luminescent Au(I) naphthalimide complexes for the detection of Polycyclic Aromatic Hydrocarbons (PAHs)

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1,8 Naphthalimides (NI) find numerous and various applications worldwide, thanks to their fluorophore and photophysical properties along with a high thermal and chemical stability and their ability to be easily functionalised[1].

The known capability of NI to form aggregates through π - π intramolecular interactions additionally to the aggregation induced emission (AIE), and the aggregation caused quenching (ACQ), has been recently investigated in our group to design NI- gold(I) complexes for the sensing of environmental contaminants, evaluating the modulation of the emission spectra [1,2].

In this scenario, the presence of gold(I) in the NI-complex is also useful to potentially trigger room temperature phosphorescence (RTP) due to the heavy atom effect, favouring the intersystem crossing and the population of the triplet excited state[3].

The focus of the project is the synthesis of two novel 1,8-naphthalimide gold(I) complexes to exploit their potential use in the molecular detection of contaminants, such as PAHs. All the obtained products have been characterized with the use of ¹H NMR, ATR FT-IR and ESI-MS. In addition, an evaluation of the luminescence properties has been performed by recording their corresponding absorption, emission and excitation spectra.

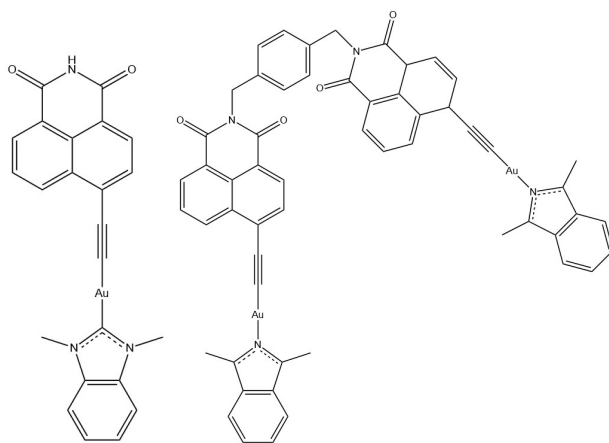


Figure 1. Au(I) Naphthalimide complexes mononuclear (left side) and dinuclear (right side)

References: [1] P. Gopikrishna, N. Meher, and P. K. Iyer, "Functional 1,8-Naphthalimide AIE/AIEE gens: Recent Advances and Prospects," *ACS Appl Mater Interfaces*, vol. 10, no. 15, pp. 12081–12111, Apr. **2018**. [2] M. Rosental et al., "Using room temperature phosphorescence of gold(I) complexes for pahas sensing," *Molecules*, vol. 26, no. 9, Apr. **2021**. [3] A. de Aquino et al., "Effect of Gold(I) on the Room-Temperature Phosphorescence of Ethynylphenanthrene," *Chemistry - A European Journal*, vol. 27, no. 5, pp. 1810–1820, Jan. **2021**.

Biodegradation of compostable and conventional microplastics by bacterial communities from granular bioreactors

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Microplastics (MP) threaten to the aquatic and terrestrial ecosystems. Several studies have reported that wastewater treatment plants (WWTPs) are one of the main sources of MP to the ocean, even though they remove up to 98% of MP from the influent. Most of these MPs are not really eliminated but end up in the sewage sludge. This sludge is normally used as fertilizer in agricultural soils, after a composting process. However, current regulation does not consider the concentration of MP in sludge before their application on natural soils. This work focused on evaluating the effect of composting on MP particles. For this, we spiked sewage sludge from a Portuguese WWTP with MP films (2 mm²) from a polyethylene terephthalate (PET) bottle and a compostable (according to the seller) bag of polyethylene (CPE), as shown in Figure 1. The experimental set-up consisted on: sludge spiked with 40 PET particles, sludge spiked with 40 CPE particles. These two treatments were repeated but inoculating a bacterial isolate from the genus *Bacillus*. Sludge with no added MP or bacterial inoculum was used as control. Samples were kept at 50°C for 60 days, and organic matter content, pH, C:N ratio, the change in the functional groups of MPs, and changes in the bacterial community were monitored monthly. Also, morphological changes on the surface of MPs were inspected using scanning electron microscopy at the end of experiment showing adherent biofilms and a fracture in MPs from the bioaugmentation treatment. Furthermore, there was some significance difference between some functional groups of MPs but not for organic matter, pH and, C:N ratio as shown in Figure 1. The 40 MPs did not affect the composting cycle opening a gate for future legislation concerning of limits of MPs for composting.

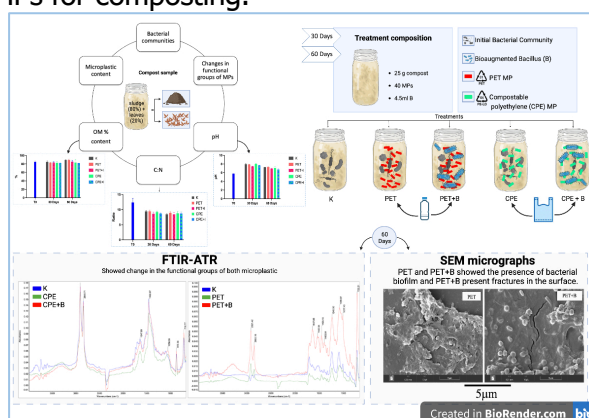


Figure 1. Scheme of the experimental setup and results. The treatment composition was 25 g of compost 40 particles of either PET or CPET MPs and 4.5ml of bioaugmented bacteria. Negative (K) controls do not include bioaugmented bacteria or the MP films

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD. This work was financed by Portuguese national funds through FCT – Fundação para a Ciências e Tecnologia, I.P., within the scope of the project PTDC/CTA-AMB/7782/2020, and through projects UIDB/04326/2020, UIDP/04326/2020 and LA/P/0101/2020. Isabel Marín Beltrán was awarded with a fellowship from the Stimulus of Scientific Employment, Individual Support 2017 Call (CEECIND/03072/2017).

Performance of advanced oxidation processes for micropollutant removal contained in urban wastewater

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Water is one of the most valuable resources in the world as it contributes greatly to domestic, industrial, and agricultural activities thereby boosting economies. It has been estimated that 70 % of useable water is being used for agricultural purposes, which has been projected to increase by 55 % by 2050 due to an increase in population and subsequently agricultural activities (Mannina et al., 2022). However, in recent times water scarcity has become a global concern and several types of research and scientific literature have indicated that wastewater reclamation and reuse is key in facing the foreseeable water scarcity head-on. Despite the effectiveness of conventional Urban Wastewater Treatment Plants (UWTP) in the removal of BOD, COD, and to some extent nutrients such as phosphorus and nitrogen, it is highly inefficient in the removal of persistent micropollutants. These micropollutants originate from pesticides, pharmaceuticals, illicit drugs, Personal Care Products (PPCPs), phthalates, agrochemicals, endocrine disruptors, polycyclic aromatic compounds, synthetic and natural hormones, and resistant microorganisms. These are collectively term as contaminants of emerging concern (CECs) due to their chronic toxicity to the environment and human health. Among several technologies and methodologies, Advanced Oxidation Processes (AOPs) have proven to be a better alternative to remediate these micropollutants. Some of the most promising AOPs are those based on the use of ultraviolet (UV) light and weak oxidants, such as hydrogen peroxide, chlorine or persulfate salts, although the operating costs of these treatments are high due to the electricity requirements for the operation of the lamps. For this reason, attempts have been made for some time to replace ultraviolet radiation with natural light from the Sun. Of the many AOPs, solar photo-Fenton have shown promising efficacies against CECs degradation and removal. In this study, solar photo-Fenton at natural pH using iron chelates treatments were performed to remove 27 CECs at 1 µg/L (each one) including pharmaceuticals, pesticides, and personal care products from different wastewater effluents from an UWTP. The aim of this project was to evaluate the feasibility of a possible new AOP (solar photo-Fenton) that uses sunlight as a source of radiation and compare it with other solar-based process (photolysis at natural pH). The basic aspects of the process were studied, such as the kinetics and mechanisms associated with the degradation of pollutants, in an experimental photochemical system at laboratory scale where solar radiation was simulated using a chamber equipped with Xenon lamp (SUNTEST CPS+, Hereaus). Also, three wastewaters with different physicochemical characteristics were tested to determine the influence of the water matrix on the process efficiency. In the photo-Fenton process, same concentration of iron and hydrogen peroxide (H₂O₂) (5 mg/L of Fe and 50 mg/L of H₂O₂) was used but three chelating agents of Fe were investigated (DTPA, EDTA and EDDS). The residual concentration of CECs was measured through the Ultra Performance Liquid Chromatography coupled to a triple quadrupole mass spectrometry Xevo TQ-S MS Detector (Waters). Residual H₂O₂ and total dissolved iron were also analyzed following spectrophotometer methods. The preliminary results revealed that the matrices with more organic matter and turbidity achieved low CECs removal in general due to the competition for hydroxyl radicals and the effect of the light scattering. Comparisons between iron complexes indicated that the stability of iron is a

key factor in the removal of CECs. Comparing the two processes, preliminary results indicated that solar photo-Fenton achieved a good performance on CECs removal.

Acknowledgments: Charles Kofi Ayi is grateful with the Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD. The authors also wish to thanks the Spanish Ministry of Science and Innovation (project PID2020-112674RB-I00, MINECO/FEDER, UE).

References: [1] López-Vinent, N., Cruz-Alcalde, A., Gutiérrez, C., Marco, P., Giménez, J., & Esplugas, S. (2020). Micropollutant removal in real WW by photo-Fenton (circumneutral and acid pH) with BLB and LED lamps. *Chemical Engineering Journal*, 379, 122416.

<https://doi.org/10.1016/j.cej.2019.122416>. [2] Mannina, G., Gulhan, H., & Ni, B. J. (2022). Water reuse from wastewater treatment: The transition towards circular economy in the water sector. *Bioresource Technology*, 363, 127951. <https://doi.org/10.1016/j.biortech.2022.127951>.

Emerging pollutants removal by advanced oxidation processes: A case of study with nanoplastics

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Nanoplastics (NPs), characterized by sizes $< 1 \mu\text{m}$, are particularly harmful since they are very likely to pass through drinking water treatment plants and can penetrate human organs and cell membranes. However, the fate of NPs in water treatment plants has been less explored compared to MPs; which is associated with the challenges of analyzing the presence of NPs in the water system [1]. Advanced Oxidation Processes (AOPs) appear as promising alternatives on account of their ability to oxidize emerging pollutants by generating hydroxyl radicals ($\bullet\text{OH}$). Catalytic ozonation would allow to achievement of higher removal rates of targetted pollutants, reduce the ozone dose and energy requirements and enhance mineralization. In this work, homogeneous catalytic ozonation by the employment of transition metal ions has been investigated for the removal of polystyrene (PS) nanoplastics. The optimization studies of the catalyst concentration, pH, and catalytic mechanisms have also been evaluated.

Nano-sized PS ($d=0,140 \mu\text{m}$) was selected as model nanoplastics due to its high proportion based on daily plastic needs and its role as the main component of plastics waste detected in water environments [2]. Ozonation experiments were carried out in a semi-continuous reactor (620 ml) under controlled temperature (20°C) and magnetic stirring (850 rpm), consisting of ultrapure water contaminated by 20 mg L^{-1} of NPs. Different concentrations of metallic ion catalysts, Fe^{3+} , Co^{2+} , Ni^{2+} , and Zn^{2+} , were prepared from salt solutions. A continuous flow of ozone (10 mg L^{-1} , $0,5 \text{ L min}^{-1}$) was established and continuously fed to the reactor for up to 120 minutes.

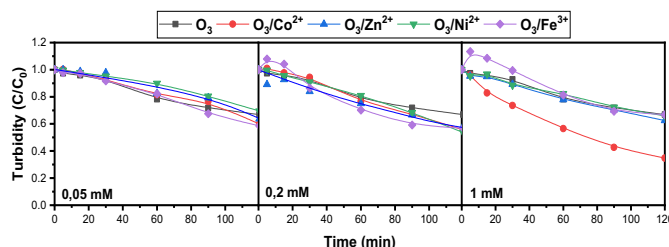


Figure 1. Turbidity (C/C_0) reduction during catalytic ozonation ($\text{pH } 3$, $[\text{PS}]=20 \text{ mg/L}$, $[\text{O}_3]=10 \text{ mg/L}$, $T=20^\circ\text{C}$, O_3 flow rate= $0,5 \text{ L/min}$) employing different concentrations of metallic ions

The single ozonation of NPs, in the absence of a catalyst, led to low turbidity reduction (33,2%) and low mineralization rate (16,1%) (Figure 1). Nevertheless, the higher ozonation performance was significantly achieved when employing Co^{2+} at a concentration of 1 mM, with obtained turbidity and mineralization were 65,2% and 69,9% respectively. As other metals showed almost similar evolution of turbidity decrease and mineralization as single ozonation, Co^{2+} (1 mM) performed at pH 3, appears as the catalyst with the most significant degradation of organic carbon in NPs. The scavenger experiments with TBA and methanol confirmed that $\bullet\text{OH}$ is responsible for NPs degradation rather than complex metal-PS formation.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

References: [1] Arenas, L.Ramizers, Gentile, S.Ramseier, Zimmermann, S., Stoll, S.; *Science of the total environment* **2022**, vol.813. [2] Y Li et al; *Chemical Engineering Journal* **2022**, vol.427

UV-assisted activation of different oxidants for wastewater remediation: feasibility and comparative study

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Due to the world's fast-growing population, industrialization has resulted in a huge need for safe and clean water. The World Health Organization and United Nations Environmental Program reveal that many countries including developing ones are under the threat of imminent health risks which are likely to be complicated and challenging because of the existence of pharmaceutically active agents in aquatic systems (Tijani et al., 2013). Water contamination by refractory substances, even at trace concentrations, may entail negative ecological implications because of the toxic and bioaccumulative properties of these compounds. Incomplete metabolism, improper disposal, or insufficient removal by treatment plants are the main causes of the release of micropollutants into the environment. Traditional wastewater treatment plants (WWTPs) do not fully remove these contaminants due to a lack of proper technologies for that purpose (Hassani et al., 2023).

Advanced oxidation processes (AOPs) are considered a promising option because highly reactive radicals such as hydroxyl and sulfate radicals generated in AOPs can effectively oxidize a broad range of emerging contaminants; other radicals such as reactive chlorine and nitrogen radicals can also play significant roles (Wang et al., 2023). This research investigates the performance of the combination of UV₂₅₄, UV₂₅₄/H₂O₂, and UV₂₅₄/Cl₂ Processes for the remediation of contaminants in terms of their efficiency and economic viability. To achieve this, oxidation experiments were conducted at the gross scale with actual wastewater effluents collected from a membrane bioreactor implemented as a secondary treatment in a WWTP near Barcelona, Spain. The wastewater spiked with a mixture of twenty-seven (27) micropollutants at trace concentrations (1 µg/L each) covering a wide range of chemical structures (and thus reactivity with oxidants involved and photoactivity towards UV 254 nm light).

The influence of different process parameters such as the applied oxidant dose and UV fluence are investigated against the UV₂₅₄/H₂O₂ process, the (mostly considered) standard UV₂₅₄-based AOP. Analysis of micropollutants was conducted by high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS). Measurement of other parameters during the experiment included the concentration of oxidants and the medium absorbance.

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Study of group VI modified max phases through HF-free methods for sustainable conversion of CO₂ via reverse water gas shift reaction

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The transformation of CO₂ into valuable products through catalytic reduction has emerged as a promising strategy to address the challenges posed by global warming and energy crises. This research covers the preparation, and catalytic behavior in the reduction of CO₂ to CO for new 2D materials such as Cr₂AlC and Mo₃AlC₂ MAX phases, and their modified derivatives. Innovative HF-free routes of preparation were performed such as Hydrothermal Alkali-treatment^[1], ultrasonic under FeCl₃^[2] and Ultraviolet radiation^[3]. To further enhance their performance, they were supported on ZnO-ZnO₂-Ga₂O₃ by an ultrasonic assisted method. All the materials were characterized using different techniques, including adsorption/desorption of N₂, XRD, SEM-EDX. The catalytic behavior in CO₂ conversion for CO production through the reverse water gas shift reaction achieving values of CO₂ conversion up to 59 %, with nearly 100 % selectivity to CO, tested at 600°C, with a reactant mixture CO₂/H₂ = 1/3 (molar ratio), 1 bar and a gas hourly space velocity of 3000 h⁻¹.

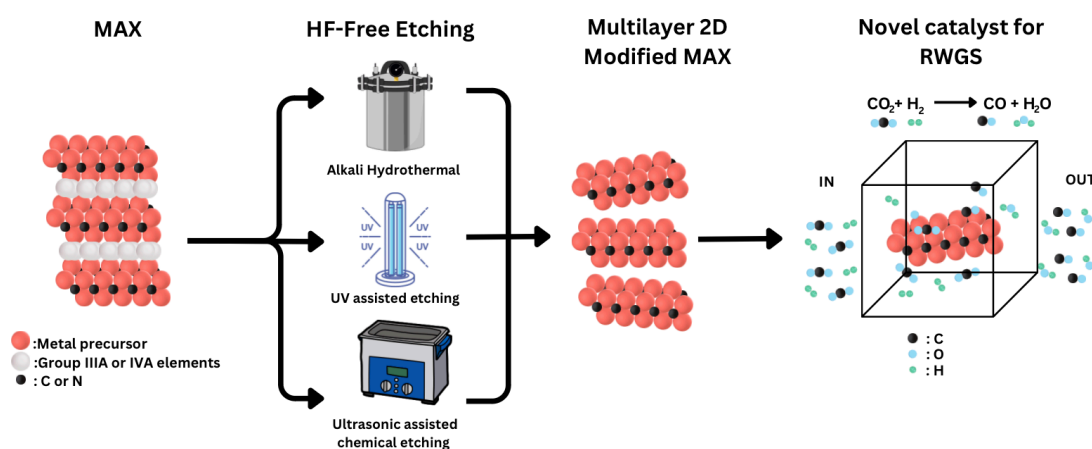


Figure 1. Graphical Abstract

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Micellar chemistry for sustainable peptide synthesis

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Peptide production stands as one of the most vital and rapidly growing sectors within the pharmaceutical industry, offering a wide array of therapeutic applications [1,2]. The conventional methods of peptide synthesis rely heavily on organic solvents, such as N,N-dimethylformamide (DMF), N-methyl pyrrolidone (NMP), and dichloromethane (DCM), leading to significant generation of hazardous waste [3]. However, their adverse effects on human health and the environment, as well as their substantial carbon footprint, have prompted the need for greener alternatives. Micellar chemistry, with water as the solvent, provides a promising alternative to traditional organic solvents, mitigating the adverse environmental impacts associated with conventional approaches [4]. In this study, commercially available surfactants in water were investigated for their potential in facilitating a simple peptide coupling reaction. Different coupling agents and reaction parameters, such as time and surfactant solution concentration, were explored. Co-solvents and binary surfactant systems were also examined to enhance reaction efficiency and selectivity. The success of the peptide coupling reactions was evaluated through product yields and analysis using proton nuclear magnetic resonance (H-NMR) spectroscopy, confirming the effectiveness of surfactant-based systems in promoting desired coupling reactions.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Solvent Assessment and Selection Aiding Tool

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Increased environmental awareness has, since the end of the 1980s, helped shift the paradigm from waste remediation to waste prevention [1]. The introduction of the green chemistry concept and the publication of the twelve principles in the 1990s has been particularly embraced by the pharmaceutical industry, where typically between 25 and 100 kilograms of waste are generated per kilogram of product (ratio known as the E-factor) [2]. In this context, several manuals and guides that intend to evaluate solvents and facilitate their selection have been released, published both by individual companies (e.g., Pfizer, GSK, AstraZeneca) and working groups (e.g., ACS GCI-PR, CHEM21).

In alignment with these efforts, a novel solvent assessment tool is proposed, tailored to suit Hovione's unique context, and integrating sustainability assessment, performance appraisal, and cost analysis into a unified framework.

Acknowledgments: We would like to express our sincere gratitude to the Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD, for their financial backing. We also wish to extend our appreciation to Hovione for the continuous assistance in the project, and are thankful to all its collaborators for their invaluable support, feedback, and dedication in advancing this initiative.

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Finding greener solvent and deprotection/cleavage reagents for solid phase peptide synthesis

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In the synthesis of peptides, solvent washings represent 80-90% of the total waste of the process, to this we have to add that they are derived from petroleum sources and are hazardous to human health and the environment [1], so it is vital to find greener alternatives. On the other hand, in the Fmoc solid phase peptide synthesis, trifluoroacetic acid (TFA) is usually employed as a deprotecting agent at concentrations around 90-95% but, TFA is an aggressive, extremely corrosive acid that can seriously injure human health, through inhalation as well as skin contact leaving hard to heal chemical burns. Peptides for medicinal use have to be freed from traces of TFA, therefore, it is imperative to replace TFA in peptide synthesis with an equally or more effective substance which would be less hazardous, less corrosive, and less environmentally dangerous.

Most acid-labile protecting groups used in the Fmoc method to mask the side chains of amino acids belong to the tert-butyl family: tert-butyl ester for carboxylic acid groups of Asp and Glu, tert-butyl ether for hydroxygroups of Tyr, Ser, and Thr, and Boc for the amino group of Lys and indole nitrogen of Trp [2,3]. Also employed are the triphenylmethyl (trityl, Trt) protecting group for the amides of Asn and Gln, imidazole ring of His, and thiol group of Cys. Third, arenesulfonyl protecting groups such as 2,2,4,6,7-pentamethyldihydrobenzofuran-5-sulfonyl (Pbf) or 2,2,5,7,8-pentamethylchroman-6-sulfonyl (Pmc) are used for the guanidino group of Arg.

In this project, eleven different peptides were synthesized manually with the formula H-Phe-AA-Gly-Gly-OH where AA stands for an amino acid: Asn, Asp, Ser, Thr, Trp, Cys, Arg, Lys, Tyr, Glu and Gln. DMF and DCM were used as solvents, for deprotection 20% piperidine in DMF was used, for coupling reactions the additives used were oxyma pure, TBEC and DIEA. Each resin with peptide was divided into different samples of 0.01 g, then cleaved with different acidic solutions (HCl or methanesulfonic acid) and were left to react at 5 different times: 45 min, 90 min, 135 min, 180 min and 24 hours. The filtered product was then evaporated to remove the acids and diluted with a solution of 1:1 acetonitrile water to be analyzed via HPLC and ESI MS, afterwards the leftover resins were treated with a TFA 95% solution for 35 mins and the filtered liquid was given the same treatment, this with the purpose of recovering any leftover peptide that wasn't cleaved initially.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Mechanochemical synthesis of API intermediates based on natural compounds

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The thesis work involved investigation of chemical transformations and their transition to mechanosynthesis method using ball-mill equipment. The work involved manufacturing of Active Pharmaceutical Ingredients and their Intermediate using mechanochemistry. Similar to catalysts, some solvents do not play role in chemical transformations. Therefore, it is possible to group solvents as participatory or non-participatory. The use of solvents consider their supply, use, treatment, and disposal leading to their financial coverage. Therefore, it is necessary to minimize their use in an industrial scale. Thus, the reactions tested mainly include Acylation, Substitution, Imine formation, and Aldol reactions. Yet, focusing on green chemistry and sustainability, the idea beyond the synthesis was to use chemicals that could be found in the nature or extracted from plants. The analysis of these compounds led to the use of various families, once the first phase reaction sets were tested. After they were observed to give quantitative conversion and high yields, it was decided to test those families including Flavanoids and Coumarins. The whole project involved the use of characterization of final products including, thin layer chromatography (TLC) and nuclear magnetic resonance (NMR). Additionally, some of the final products were theoretically proven to be biologically active and suitable for the manufacturing of new APIs.

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Designing a long-lasting corrosion inhibitor for liquid oscillating dampers in wind turbine towers

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Wind turbines are complex structures that harness wind energy to generate electricity. As wind speeds increase, the aerodynamic forces acting on the turbine blades also increase, resulting in vibrations and oscillations. These vibrations can lead to fatigue damage, reduced performance, and even structural failures over time. To mitigate these issues, oscillating dampers are employed in wind turbines. Liquid oscillating dampers play a critical role in mitigating structural vibrations induced by wind loads, and their performance can be significantly affected by corrosion-induced degradation.⁽¹⁾ The purpose of this research is to investigate corrosion protection techniques for liquid oscillating dampers.

The liquid damper contains 30% CaCl₂ in water in a carbon steel tank and inhibitors should protect carbon steel against the destructive effects of CaCl₂ solution. For reaching that goal different kind of corrosion inhibitor was blended several compounds such as ammonium molybdate, sebacic acid, tolyl triazole, benzoic acid, isonanoic acid. Solutions with different percentages have been prepared⁽²⁾ and tested to check the their stability and effectivity, compatibility and durability. Six different mixtures have been prepared but four were rejected in the compatibility and stability tests. The other two are currently being tested and after passing this stage, they will be checked for effectiveness on carbon steel, as the reservoir material for the liquid dampers

Acknowledgments: I would like to express my deepest gratitude to the people behind EMMC-ChIR, (grant agreement nr 619824-EMJMD) for giving me this incredible opportunity to go on a journey of obtaining the foremost knowledge and skills in the area of chemical innovation and regulation. The present research project would not have been possible without the considerable support of Comercial Química Massó in Spain.

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Metal-Organic Frameworks (MOFs) of extended triphenylenes for an intended green catalysis

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Metal-organic frameworks are nanomaterials assembled between inorganic metallic nodes and organic bonds, being widely investigated in the heterogeneous catalysis field due to the high surface area and porosity [1,2]. Specifically, the research is focused on 2D MOFs functionalized with amine groups due to their advantages such as rendering active sites because of their basic properties, or their possibility of catalyst recovery [3].

This work will be focused on the catalyst properties of different MOFs extended triphenylenes functionalized with amines: 2,3,6,7,10,11-hexaaminotriphenylene (**HATP**), 2,3,6,7,10,11-hexakis(tert-butylamine) triphenylene (**HTATP**), and 2,3,6,7,10,11-hexakis(methylamine)triphenylene (**HMATP**). HTATP and HMATP will be synthesized through a cross-coupling reaction C-N catalyzed by palladium (Buchwald-Hartwig method), and copper (Ullmann method). Both will be characterized by ^1H and ^{13}C NMR.

Regarding the amine ligand synthesis, metallic salts of Pd (II), Cu (II), and Ni (II) will react individually with these three extended triphenylenes. The MOFs characterization is based on the application of different techniques such as infrared spectroscopy (IR) to evaluate the presence of functional groups, powder X-ray diffractometer (PXRD) to evaluate the crystallinity, and scanning electronic microscopy (SEM) to determine the morphology (Figure 1).

The last step is based on their use as catalysts in the reaction Suzuki-Miyaura with 4-bromoanisole and phenylboronic acid as reagents. The synthesis will take place in natural deep eutectic solvents (NADES) at 80°C to ensure adequate viscosity to easily transfer matter.

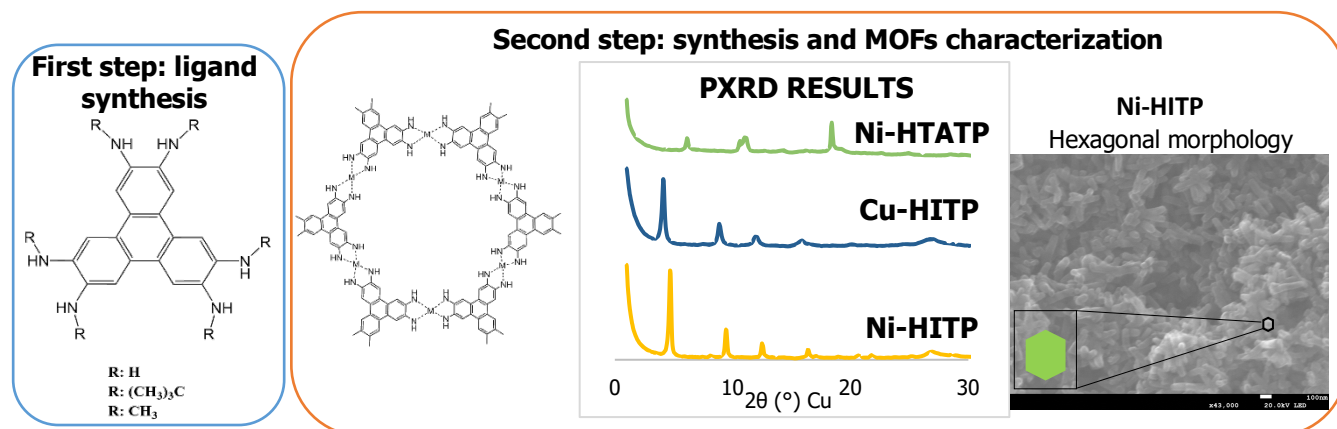


Figure 1. Synthesis and MOFs characterization scheme.

Acknowledgments: ANP thanks to Massó Foundation for scholarship funding.

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Evaluation of reinforcement of polylactic acid (PLA) for 3D printing: properties and risk assessment

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The growing focus on sustainable and biodegradable materials drives this study's investigation into the application of bamboo fibers (BF) and Single-walled carbon nanotubes (SWCNT) as reinforcements in a polylactic acid (PLA) polymer matrix for 3D printing purposes. PLA, a biobased and biodegradable biopolymer, is a widely employed thermoplastic in the field of 3D printing due to its excellent rheological properties, enabling efficient printing processes. However, 3D printed PLA pieces faces limitations in terms of mechanical properties such as impact resistance and toughness¹. It has been seen that incorporating natural fibers as reinforcement holds the potential to enhance the mechanical behavior of PLA-based composites².

In addition to evaluating the mechanical properties and performance of the BF and SWCNT reinforced PLA composites, this study places emphasis on the safety aspects. The generation and release of airborne particles during the filament extruding and 3D-printing manufacturing processes is quantified. Mechanical and aging stresses are applied to simulate real-use conditions, allowing the examination of potential particle release into the environment and the subsequent potential impacts. The aging process also aims to investigate the material's ability to retain its mechanical properties over time, ensuring long-term durability and performance. Preliminary results indicate that the sieving process releases relatively higher concentrations in terms of particle number. However, in compliance with regulatory standards, the released particle concentrations are not a cause for significant concern. Nonetheless, considering the shape and long-term inhalation risks associated with these particles, a risk assessment will be conducted combining literature review and the exposure results. This assessment aims to ensure the safe usage of BF and SWCNT reinforced PLA composites in 3D printing applications, prioritizing the well-being of users and the environment.

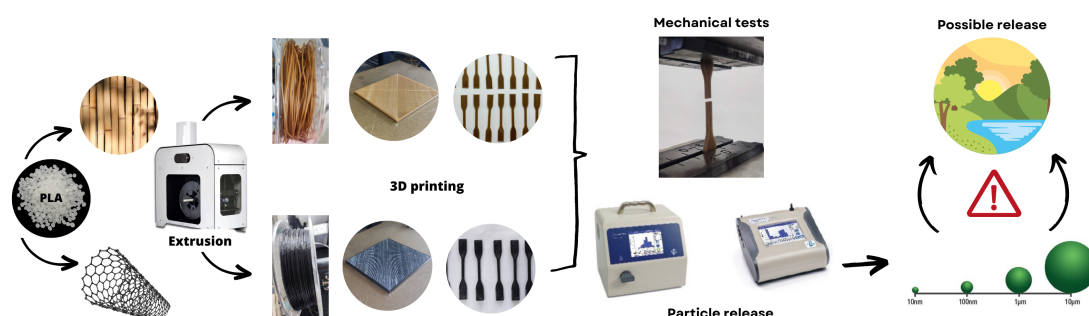


Figure 1. Methodology of the study.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Application of the New CLP Hazard Classes to the European chemical industry and its impact on the external trade with the USMCA economic region.

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The main objective of chemical regulation is protecting human health and the environment from the risks posed by chemicals. This process is dynamic. As new scientific evidence appears, regulations worldwide are usually updated.

In the European Union, one of the most important regulations governing chemicals is Regulation (EC) No 1272/2008 on the classification, labelling, and packaging of substances and mixtures (CLP).

The CLP regulation sets out the criteria to determine whether a chemical substance or mixture displays properties that lead to a hazardous classification. Generally, the classification process involves gathering all the available information about the substance or mixture to compare it with the criteria laid down in CLP. If the information collected meets the criteria, a certain hazard class and category are assigned to the chemical.

In 2022, the European Commission published a Delegated Regulation to amend CLP. The Delegated Act introduced new hazard classes and criteria for classification that entered into force on April 20th, 2023.

These new hazard classes are:

- Endocrine disruptors (ED) for human health or the environment
- Persistent, bioaccumulative, and toxic (PBT); very persistent and very bioaccumulative (vPvB)
- Persistent, mobile, and toxic (PMT); very persistent and very mobile (vPvM) [1].

The addition of new hazard classes was triggered by evidence that substances and mixtures with these properties pose a concern to public health and the environment e.g., exposure to endocrine disruptors can lead to certain disorders in humans, among others birth defects, developmental, reproductive, or neurodevelopmental disorders, cancer, diabetes, and obesity. In the environment, substances with PBT and vPvB properties do not easily break down and tend to accumulate in living organisms across the food web [2].

Nonetheless, the new hazard classes represent a divergence from the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) established by the United Nations and implemented in at least 72 countries, including the most important economic partners of the EU. The discrepancy with other main global players is expected to last some years, therefore, the present work discusses the impact of this divergence on the external trade with the USMCA economic region composed of the United States, Mexico, and Canada.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

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Isolation and identification of bioactive compounds from microalgae

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Microalgae are considered to be an untapped resource. They display high photosynthetic efficiency, tuneable growth and composition, they capture CO₂ and require relatively low amounts of water for their cultivation. Also, only less than 10% of the estimated microalgal species have been described. However, the production of microalgal products is still in a technological early stage, where economic feasibility limits their entrance to the markets. The extraction of high-value compounds from microalgae is a key step in the innovation pathway to completely capture the value of the microalgal biomass [1].

This work is focused on the screening of bioactive compounds present in *Tetraselmis striata* CTP4 (Figure 1, left). This strain was isolated from samples collected in a marsh area (Ria Formosa) in Algarve, Portugal. It has already showed potential for several market applications, and it has also been successfully cultivated in large scale production [2], [3].

Following a 'funnel approach' (Figure 1, right), the microalgal biomass was analysed through extractions, high throughput assays, and HPLC fractionation. The results confirmed the antioxidant activity of *T. striata* CTP4 and unveiled its antihypertensive activity. Next steps will try to finally identify the individual compounds responsible for these bioactivities through LC-MS analysis.

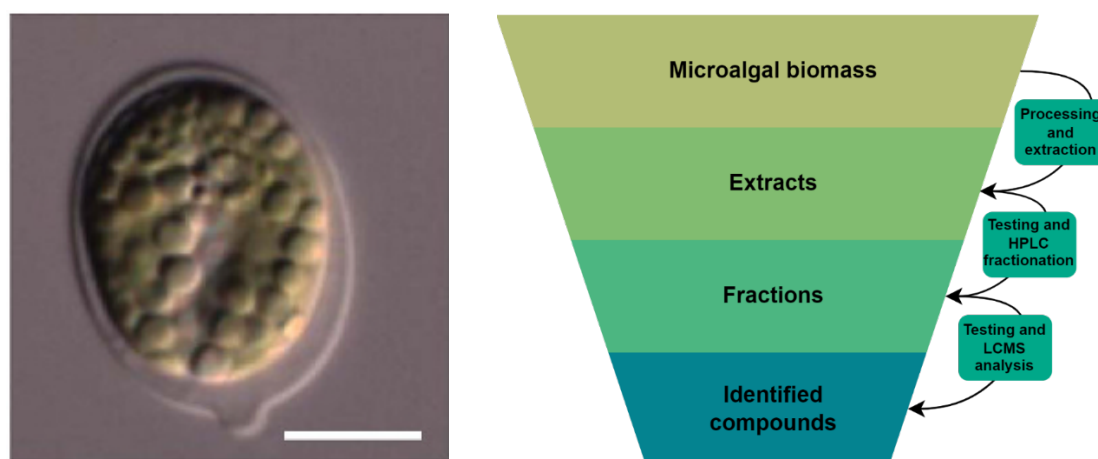


Figure 1. *T. striata* CTP4 under the microscope (left, from [3]). Funnel approach applied during the screening (right)

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Exploring the medicinal halophytes *Limonium algarvense* and *Polygonum maritimum* as sources of cosmetic ingredients

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Due to the relevance of cosmetics in modern life, the cosmetic industry is constantly searching for innovations, especially novel natural active ingredients that meet the ever-changing consumer's expectations. Lately, marine organisms have begun to be used as sources of novel ingredients to develop increasingly innovative products, including halophyte species, such as *Limonium algarvense* Erben (sea lavender) and *Polygonum maritimum* L. (sea knotgrass), found along the Algarve coast. Hence, this work prepared and evaluated innovative herbal extracts containing mixtures of sea lavender and sea knotgrass at different ratios, aiming their valorisation as sources of novel cosmetic ingredients. For that, aqueous extracts were evaluated for their chemical and functional properties, including antioxidant activity on DPPH•, ABTS•⁺, O²⁻, and HO• radicals, chelating activity on copper, and inhibition of enzymes related to cosmetic uses, namely tyrosinase, lipase and elastase. All samples had relevant activity as radical scavengers, being the sea lavender extract the most active on DPPH• and O²⁻ radicals (EC₅₀ = 0.155 mg/mL and 0.219 mg/mL, respectively). The mixtures at 1:3 ratio showed a higher scavenging activity on ABTS•⁺ (EC₅₀ = 0.640 mg/mL) and had the best copper chelating activity (EC₅₀ = 0.533 mg/mL) among all. Contrastingly, the mixture at 3:1 ratio had the best performance over HO• radical (EC₅₀ = 0.063 mg/mL). Regarding the enzymatic inhibitory assays, whilst the sea lavender extract had the best performance on tyrosinase inhibition (EC₅₀ = 0.183 mg/mL), the sea knotgrass extract was the only one showing an inhibitory activity towards elastase (EC₅₀ = 12.2 mg/mL). None of the tested extracts showed activity over lipase. Analysing further, the 1:3 mixture showed an additive effect (SE = 1) on the copper chelation, whereas and the mixture at 3:1 ratio had a synergistic effect on the HO• radical scavenging activity (SE = 0.2). All the other extracts had SE values over 1, meaning an antagonistic effect. The extracts were analysed by liquid chromatography – high resolution mass spectrometry. A total of 300 features were identified and flavonoids constituted the major chemical class in the mixtures. Overall, the results indicate that the sea lavender extract, and their mixture with sea knotgrass at 1:3 and 3:1 ratios are suitable sources of active compounds for the cosmetic industry given their performance as radical scavengers, metal chelators, as well as anti-wrinkles and anti-hyperpigmentation properties.

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Synthesis of several gold nanoparticle decorating Cu_{2-x}Se and Ag_2Se hetero structure nanoparticles for photothermal therapy

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The plasmonic behaviour of nanostructured materials has ignited intense research for the fundamental physics of plasmonic structures and for photothermal effect-based biomedical applications. The interaction of plasmonic modes from two different materials, namely vacancy-doped semiconductors, and metals, particularly, those that integrate gold nanoparticles, is gaining attention due to the unique phenomena that can be observed from the combination of these two inherently distinct plasmonic modes. The present study is carried out to synthesis multiple gold nanoparticles attached to copper and silver chalcogenide nanoparticles in the form of colloidal nanomaterials with controlled composition. The synthetic approach started from the preparation of gold, Cu_{2-x}Se and Ag_2Se nanoparticles. The two strategies were used to synthesis the desired hybrid nanostructure. The first strategy was employed by mixing a solution of pre-synthesized Cu_{2-x}Se and Ag_2Se with Au (III)DDA in toluene. The second method was conducted by combining premade Cu_{2-x}Se and Ag_2Se with pre-synthesized gold nanoparticle in toluene. The different stoichiometric ratio of Au (III)DDA, pre-synthesized AuNPs, Cu_{2-x}Se and Ag_2Se nanoparticles were simply mixed at room temperature and the formation of several gold nanoparticle decorating hybrid Cu_{2-x}Se and Ag_2Se nanostructure were studied by withdrawing aliquots from reaction flask at certain time interval. The composition and concentration of gold, Ag_2Se and Cu_{2-x}Se NPs solution was determined by inductively coupled plasma-atomic emission spectroscopy (ICP-AES). The morphology and size of the synthesised nanoparticle was examined by Transmission electron microscope. The optical characterization of AuNPs was carried out by UV–vis spectrophotometer and the optical absorbance of Ag_2Se and Cu_{2-x}Se were measured by NIR scanning spectrophotometer. The crystallographic structure of nanoparticles was characterized by X-ray diffraction analysis. The elemental mapping of nanocomposites was done by EDX.

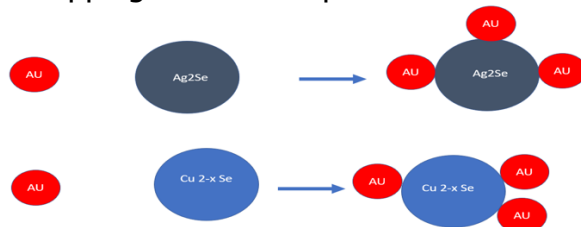


Figure 1: Shows Silver and copper chalcogenide-based semiconductor hybrid NPs containing several gold nanoparticles.

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Determining the conformational plasticity of choline trimethylamine-lyase from *Klebsiella pneumoniae*

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Choline Trimethylamine-Lyase (CutC) is an enzyme present in the gut microbiota with the ability to cleave the C-N bond of choline to produce trimethylamine (TMA). This metabolite is further oxidized into trimethylamine-N-oxide (TMAO) in the liver and is associated with a higher risk of developing metabolic and cardiovascular diseases [1]. The ultimate goal of this research is to design an inhibitor of CutC to reduce the formation of TMA. However, due to the novelty of the target, we first need to understand the dynamics of the system. Previous studies have been performed by members of the Computational Biology, Chemistry & Gastronomy (CBCG) group, providing molecular dynamics (MD) simulations of CutC from *Desulfovibrio alaskensis* G20 and *Klebsiella pneumoniae* microorganisms, since the crystallographic structures of CutC from these two microorganisms are showing different conformational behavior between the ligand-free (apo) and the ligand-bound (holo) states. Unexpectedly, the choline-bound state of CutC from *D. alaskensis* G20 does not show an effect on the plasticity conformation of CutC in comparison to the ligand-free enzyme [2]. In the case of *K. pneumoniae* the analysis is more complex since the X-ray structures of apo state is not complete.[3] Homology modelling technique was used to obtain a complete 3D model of CutC protein. In this work, we show the results of MD simulations of CutC from *K. pneumoniae*, in the apo and holo states from the 3D structure obtained from SWISS-MODEL server [4], to determine the conformational plasticity of CutC in *K. pneumoniae* and determine the structural differences between the CutC from both microorganisms.

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Production of Pullulan hydrogels using trisodium trimetaphosphate as gelling agent - Study of rheological properties and food grade nanoemulsion release kinetics

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Pullulan is a commercially available highly water-soluble polysaccharide purified from the fermentation medium of the fungus-like yeast *Aureobasidium pullulans* (originally *Pullularia pullulans*) [1]. Pullulan products are edible and biodegradable [2]. Trisodium trimetaphosphate (TSMP) is of special interest as crosslinking agent as it is non-toxic. The formation of pullulan gels and their rheological properties have been scarcely studied in the bibliography [3]. In this communication, the composition variables to obtain pullulan gels, such pullulan/KOH ratio and pullulan/TSMP ratio have been studied. Rheological behaviour of the gels at different compositions including the kinetics formation over time and the influence of temperature are studied.

The use of gels based on biopolymers such alginate, chitosan and others have been widely studied as shell materials for the incorporation of different functional foods. In the present work, carvacrol- main molecule of oregano essential oil- has been selected as an active component to enrich food due to strong antimicrobial and antioxidant properties. As carvacrol has a strong taste and low solubility in aqueous media, the way to add it can be as gelled oil-in-water nanoemulsion pullulan gel. Pullulan gels have not been deeply studied, and they have great potential to be used to encapsulate different kind of nutraceutical compounds. The main advantage of pullulan gels is their non-animal origin and they high transparency. In contrast, gelation time is slow, so, preliminary studies should be done using the bulk gel.

Once the composition variables to form the pullulan gel are set, one-step nanoemulsion loaded gel is obtained comparing its properties with the gel without nanoemulsion. The one-step nanoemulsion loaded gel is obtained by low-energy nanoemulsification method. A phase inversion composition (PIC) method is used. Nanoemulsion is prepared in the carvacrol/medium chain triglycerides-(oleic acid-potassium oleate/ Tween 80 ®)-pullulan/TSMP system.

The carvacrol-loaded pullulan gel release kinetics is studied. Several release kinetics models have been fitted to experimental data in order to study the release behaviour in order to determine the suitability of the gels as an additive for food preserving.

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