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6th International Conference on Risk Assessment of Pharmaceuticals in the Environment

20-21 October 2025

University of Aveiro, Portugal

ICRAPHE

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Welcome Message

Pharmaceuticals are a fundamental pillar of health for humans and other animals. However, beyond their undeniable benefits, they are increasingly recognized as significant microcontaminants, ubiquitously present in various environmental compartments at trace yet potentially impactful levels. Over the past few decades, this multidisciplinary challenge has attracted growing scientific attention, yet much remains to be discovered.

In 2016, the 1st International Conference on Risk Assessment of Pharmaceuticals in the Environment (ICRAPHE) was organized in France. Since then, ICRAPHE has become a privileged forum where experts from diverse fields of research related to this environmental issue gather to discuss the latest advances in the area.

The Organizing Committee of the 6th ICRAPHE is pleased to continue this sequence of events, bringing together scientists from 15 countries (3 continents). This edition features 3 plenary and 4 keynote lectures, 26 oral presentations, and 39 poster communications. All these contributions highlight the latest scientific achievements in analytical technologies that enable faster, easier, and more sensitive detection of pharmaceuticals in complex environmental matrices; cost-effective and sustainable treatment and remediation strategies for contaminated environments; and studies on the effects of pharmaceuticals on non-target organisms, ranging from ecological consequences to comprehensive risk assessments.

The Organizing Committee would like to express its sincere acknowledgement to all authors who submitted their work to this conference, making this Book of Abstracts and this event possible through their excellent contributions. Special thanks are also extended to the institutions that supported this event and to our valuable sponsors.

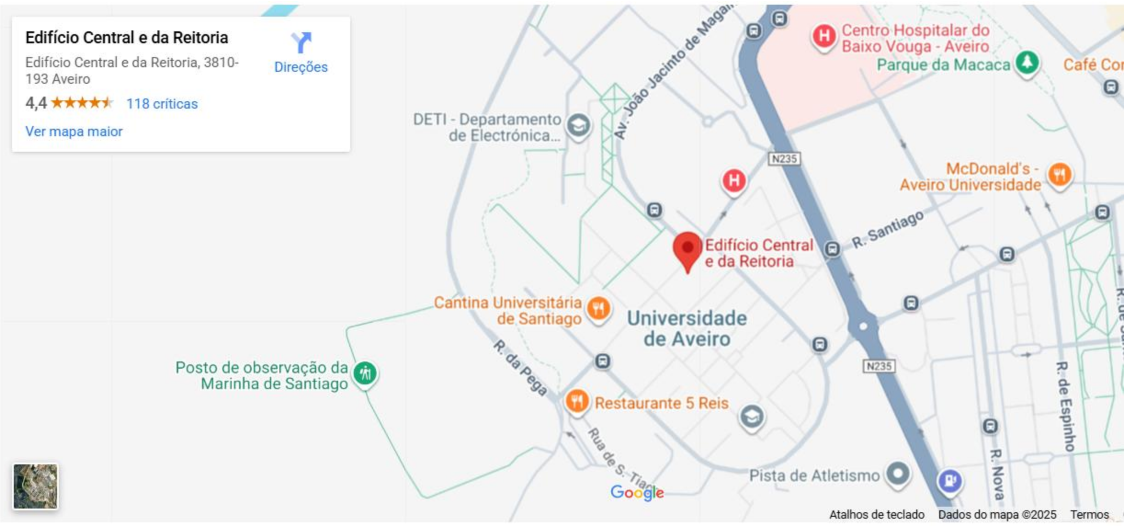
Welcome to the 6th ICRAPHE!

The Organizing Committee

Congress Information

Conference Venue

The meeting will be held in Auditório Renato Araújo, Edifício Central e da Reitoria, Universidade de Aveiro, 3810-193 Aveiro.



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Tess Goessens, Ghent University

10:25 OC2 | *Water fleas as “canaries in the coal mine” for the detection of pharmaceuticals in the environment*

Flavia Melati Chiappara, Dublin City University

10:40 OC3 | *Environmental quantification and fate of therapeutic modified oligonucleotides in mixed liquor suspended solids*

Vanessa Maybruck, University of Colorado Boulder

10:55 Coffee-break

SESSION 2 | Chair: Damià Barceló

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Rudolf J. Schneider, BAM Federal Institute for Materials Research and Testing

11:50 OC4 | *Lessons Learned from Two Decades of Research on Uncovering Emerging Contaminants and their Ecological Impacts*

Diaga S. Aga, University at Buffalo

12:05 OC5 | *Fabrication of an electrochemical sensor based on nanoclusters with carbon nanotubes for the determination of ethylmorphine*

Merve Yence, Lokman Hekim University

12:20 OC6 | *Nanomaterials-Supported MIP-Based Electrochemical Sensor for the Determination of Lenalidomide: Application to Environmental Matrices*

Farah Elbarghathi, Ankara University

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14:50 OC7 | *From powder to beads: synthesis and shaping of an imine-linked triazine porous organic polymer for antibiotic remediation from water*

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15:05 OC8 | *The Investigation of Simultaneous Nitrate and Pharmaceuticals Removal from Wastewater Treatment Plant Effluents through Sulfur-Based Autotrophic Denitrification Processes*

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15:35 OC10 | *Removal of venlafaxine from water through carbon adsorbents produced from spent brewery grains*

Angelica R. Zizzamia, University of Basilicata

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André Pereira, University of Coimbra

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Ahmet Cetinkaya, Ankara University

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10:05 OC16 | *The Effects of Ciprofloxacin on Red Sea Sponge Stylissa carteri: Implications of Antibiotic Pollution from Aquaculture*

Sofia C. Walzer, King Abdullah University of Science and Technology

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16:10 OC24 | *The Need for an Early-Stage Sustainability Assessment Methodology*

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PL3. Rosa Freitas

Pharmaceutical Pollution Meets Climate Pressure: Aquatic Ecosystems at a Crossroads

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Water fleas as “canaries in the coal mine” for the detection of pharmaceuticals in the environment

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OC18. Ana L. Patrício Silva

Microplastics as Vector for Pharmaceuticals: Analytical Challenges and Ecotoxicological Risks in Aquatic Systems

OC19. Emma Rowan

New Approach Methodologies predict pharmaceutical pollution

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P3. Filomena Lelario

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P25. Igor E. Oliveira

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Abstracts

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Lectures

PL1

Advances and Challenges in Molecularly Imprinted Electrochemical Sensors for Environmental Applications

Sibel A. Ozkan[1*]

[1]*Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye*
**ozkan@pharmacy.ankara-edu.tr*

Developing rapid, cost-effective, and "green" approaches to achieve environmental sustainability is currently one of the most important issues for addressing environmental pollution problems.

Molecular imprinting technology is a creative method that enables synthetic biorecognition gaps to imitate real biological derivatives like antibodies, receptors, enzymes, etc. After removing the target analyte, synthetic cavities enable the recognition and selective rebinding of the template. In this case, molecular imprinting technology offers biosimilar receptors with higher specific affinities and better stability than natural receptors and biomolecules [1]. Although stable and durable MIPs seem relatively easy to create to achieve maximum efficiency, some optimization parameters should be considered, such as appropriate functional monomer and crosslinker, and optimal ratios between functional monomer, template, and crosslinker [2].

Green analytical chemistry (GAC) aims to make analytical techniques less harmful to the environment and more human-friendly by reducing or eliminating toxic chemicals/reagents, using energy-efficient equipment, and using miniaturized and automated methods. Sustainability is the underlying approach to the GAC. There is an evolution towards more environmentally friendly components in an analysis process, from synthesis and analysis processes to the tools used. Thanks to these steps, minimizing waste generation and not creating harmful waste will be the most important output of GAC for the environment and human health in the long run It was reported that template monomer interactions are realized through non-covalent interactions such as van der Waals forces, hydrogen bonds, and dipolar interactions [1, 2].

MIP-based electrochemical sensors and miniature electrochemical transducers can detect target analytes in situ. Thanks to superior chemical and physical stability, low-cost manufacturing, high selectivity, and fast response, MIPs have recently become an interesting field. The increase in environmental awareness and stricter regulation for the use of chemicals and economic competitiveness are challenging the scientific community and industry to explore greener strategies in their processes, preventing pollution and reducing waste while maximizing the efficiency of the processes, and that can only be achieved by the application of the green chemistry and engineering principles.

[1] L. Uzun, A.P.F. Turner, Molecularly-imprinted polymer sensors: realising their potential, Biosens. Bioelectron. 76 (2016) 131e144.

[2] K. Graniczkowska, M. Pütz, F.M. Hauser, S. De Saeger, N.V. Beloglazova, Capacitive sensing of N-formylamphetamine based on immobilized molecular imprinted polymers, Biosens. Bioelectron. 92 (2017) 741e747.

PL2

Intensification of Advanced Oxidation Processes in Multi-Scale Reactors for the Removal of Pharmaceuticals Residues in Water

Gianluca Li Puma[1*]

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Advanced oxidation processes (AOP), such photolysis, UV-H_2O_2, solar photo-Fenton, photocatalysis and photoelectrocatalysis are oxidative processes based on the formation of powerful radical species capable of degradation of persistent pharmaceuticals residues in surface water, groundwater and wastewater.

In this presentation, the optimisation and intensification of degradation of persistent pharmaceutical residues in water such as antidepressants, antibiotics, oestrogens, antiviral, antiretrovirals, antifungal and illicit drugs will be discussed in multi-scale chemical, photochemical and photoelectrochemical reactors including a LED-Internet of Things assisted solar packed bed photocatalytic reactor system [1], microcapillary and array film photoreactors [2-5], pilot-scale solar photocatalytic reactors [6-7] and full-scale solar photo-Fenton raceway reactors [8].

The intensification of pharmaceutical removal in such reactors is realized through efficient reactor design and operation, in which mass transport, radiation transport and fluid-dynamics are holistically analysed using computation fluid-dynamics approaches.

[1] Kubiak, A; Lima, S.; Li Puma, G. Adaptive bioinspired Light Emitting Diode-Internet of Things (LED-IoT) assisted solar packed bed photocatalytic reactor system for naproxen removal from real wastewater matrices, *Chemical Engineering Journal* 522 (2025) 67518.

[2] Yusuf, A.; Garlisi, C.; Peralta Muniz Moreira, R.; Li Puma, G.; Palmisano, G. Multiphysics computational fluid dynamics (CFD) modelling of diclofenac amide removal by photocatalytic oxidation on Fe-TiO2/N-TiO2 thin films microreactor, *Chemical Engineering Science*, 274 (2023) 118662.

[3] Reis, N.M.; Li Puma, G. A novel microfluidic approach for extremely fast and efficient photochemical transformations in fluoropolymer microcapillary films, *Chemical Communications*, 51 (2015) 8414.

[4] Russo, D.; Siciliano, A.; Guida, M.; Andreozzi, R.; Reis, N.M.; Li Puma, G.; Marotta, R. Removal of antiretroviral drugs stavudine and zidovudine in water under UV254 and UV254/H_2O_2 processes: Quantum yields, kinetics and ecotoxicology assessment' *Journal of Hazardous Materials*, 349 (2018) 195.

[5] Moreira, R.P.M.; Li Puma, G. CFD modeling of pharmaceuticals and CECs removal by UV/H_2O_2 process in helical microcapillary photoreactors and evaluation and OH radical rate constants, *Chemical Engineering Journal*, 415 (2021) 128833.

[6] Wang, D.; Mueses, M.A.; Colina-Marquez, J.; Machuca-Martinez, F.; Grčić, I.; Moreira, R.P.M.; Li Puma, G. Engineering and modeling perspectives on photocatalytic reactors for water treatment, *Water Research*, 202 (2021) 117421.

[7] Li Puma, G.; Puddu, V.; Tsang, H.K.; Gora, A.; Toepfer, B. Photocatalytic oxidation of multicomponent mixtures of estrogens (estrone (E1), 17β-estradiol (E2), 17α-ethynylestradiol (EE2) and estriol (E3)) under UVA and UVC radiation: Photon absorption, quantum yields and rate constants independent of photon absorption', *Applied Catalysis B: Environmental*, 99 (2010) 388.

[8] Moreira, R.P.M.; Cabrera Reina, A.; Soriano Molina, P.; Sanchez Perez, J.A.; Li Puma, G. Computational fluid dynamics (CFD) modeling of removal of contaminants of emerging concern in solar photo-Fenton raceway pond reactors, *Chemical Engineering Journal*, 413, (2021) 127392.

PL3

Pharmaceutical Pollution Meets Climate Pressure: Aquatic Ecosystems at a Crossroads

Rosa Freitas[1*]

[1]*Department of Biology & CESAM, University of Aveiro, Portugal*
**rosafreitas@ua.pt*

Pharmaceuticals are continuously detected in aquatic systems worldwide, raising concerns about their long-term ecological consequences. Research conducted by Rosa Freitas and her team at the University of Aveiro has systematically addressed the bioaccumulation, toxicity mechanisms, and interactive effects of these contaminants in aquatic wildlife, with a particular focus on invertebrate models such as mussels, clams, and polychaetes. Experimental studies have demonstrated that exposure to common pharmaceuticals, including non-steroidal anti-inflammatory drugs, antihistamines, anticonvulsants, and synthetic hormones, can induce significant physiological and biochemical disturbances even at environmentally relevant concentrations. Documented effects include oxidative stress, disruption of antioxidant defenses, altered metabolic performance, neurotoxicity, and histopathological damage to key tissues (e.g. gills and digestive glands). Importantly, results indicate that climate change stressors such as elevated temperature, salinity shifts, and acidification often exacerbate pharmaceutical toxicity, highlighting the need for multi-stressor approaches in ecotoxicology. The group has further contributed to understanding mixture toxicity, biotransformation processes, and the capacity for recovery following exposure, providing mechanistic insight into species-specific sensitivities. This integrative perspective, combining physiology, biochemistry, and environmental stress ecology, reveals that pharmaceuticals act as subtle yet pervasive drivers of change in aquatic organisms, potentially compromising population resilience and ecosystem services. Overall, this research emphasizes the importance of incorporating pharmaceuticals into regulatory frameworks and risk assessment models, while accounting for the compounding influence of global change. By bridging fundamental and applied perspectives, it provides critical tools for advancing ecotoxicological monitoring and protecting aquatic biodiversity.

Keynotes Lectures

KN1

How Can Antibodies Help Us in the Risk Assessment of Pharmaceuticals in the Environment?

Rudolf J. Schneider[1,*]

[1]*BAM Federal Institute for Materials Research and Testing, 12205 Berlin, Germany*
** rudolf.schneider@bam.de*

The widespread use of pharmaceuticals has led to their persistent presence in various environmental compartments, raising concerns about ecological and human health risks since they pose a significant threat to non-target organisms and human health, necessitating robust methods for environmental risk assessment.

Traditional analytical methods, such as liquid chromatography-mass spectrometry (LC-MS), offer high sensitivity and specificity but are often resource-intensive, require complex sample preparation, limiting their applicability for large-scale or real-time monitoring. In this context, antibody-based analytical techniques present a promising complementary approach for the detection and quantification of pharmaceutical residues in environmental matrices.

Antibodies, due to their high specificity and affinity, enable the development of immunoassays such as ELISA, lateral flow assays, fluorescence-based formats, and electrochemical sensors that are rapid, cost-effective, and adaptable to field conditions. These methods can be tailored to target a wide range of pharmaceutical compounds, including antibiotics and endocrine disruptors. Moreover, antibody-based assays facilitate high-throughput screening and can be integrated into portable platforms for on-site analysis, thereby enhancing temporal and spatial resolution in environmental monitoring.

This presentation explores the potential of antibodies in environmental risk assessment, focusing on their application in detecting trace levels of pharmaceuticals in water, soil, and biota. They are presented as a complementary and powerful tool for rapid, cost-effective screening in the lab and that also can be deployed for on-site analysis in the field.

The talk also discusses recent advances in antibody engineering, multiplexing capabilities [1], and the integration of immunoassays with sensor technologies [2].

Case studies illustrate how immunoanalytical data can help in finding potential contamination hotspots [3], hazard identification, pollution source tracking, and the generation of crucial data for predictive models on environmental fate and effects. Antibody-based methods can also help in early warning systems and the evaluation of mitigation strategies, contributing to a more comprehensive and proactive risk assessment framework, eventually to regulatory decision-making, ultimately aiding in the protection of ecosystems and public health.

[1] Carl, P., et al. *Anal. Chem.* 2019, *91*, 12988-12996
[2] Raysyan, A., et al. *Anal. Bioanal. Chem*. 2021, *413*, 999–1007
[3] Bahlmann, A., et al. *Chemosphere* 2012, *89* (11), 1278-1286

KN2

Electrobioremediation of pharmaceuticals in urban and industrial wastewater: the METFILTER® modular solution

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Electrobioremediation is an emerging branch of biotechnology that uses electrochemical methods to improve the biodegradation capabilities of microorganisms (Tucci et al., 2021). Wastewater has been the primary testing environment for Microbial Electrochemical Technologies (MET), which address the common limitation of low electron acceptor availability by providing an electrode to receive electrons from pollutant metabolism.

So far, the most prominent electrobioremediation approach in wastewater treatment is the METfilter® system, which incorporates electrochemical principles into constructed wetlands. This hybrid design uses conductive carbon-based materials to boost microbial pollutant oxidation and drastically reduces the footprint—requiring as little as 50 m² to treat wastewater from 1000 people. The system has been developed into modular, plug-and-play units that can also treat industrial wastewater from sectors such as oil & gas, food & beverage, and pharmaceuticals.

Micropollutants like pharmaceuticals often resist breakdown in conventional biological treatment. Electrobioremediation overcome this limitation by linking microbial respiration to solid electron acceptors (e.g., electrodes) during pollutant metabolism. METfilters have effectively removed micropollutants in horizontal flow setups, and notably enabled stereoselective biodegradation of compounds like propranolol. Effluent detoxification was confirmed using bioassays with Daphnia magna and Raphidocelis subcapitata.

The enhanced degradation of complex pollutants may stem from unique microbial synergies within the conductive bed. A redox-interconnected community can optimize metabolic resource use and facilitate electron exchange, promoting oxidation or reduction of diverse functional groups.

A modular METfilter system has been successfully piloted for removing high pharmaceutical loads from real industrial wastewater at a production facility. Performance results will be presented and discussed.

KN3

Veterinary Pharmaceuticals in Aquatic Environments: Risks, Detection, and Sustainable Solutions

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Veterinary pharmaceuticals are essential for maintaining animal health, but their widespread use can lead to environmental residues that threaten ecosystems and public health. Highest-priority critically important antibiotics (HPCIAs), including fluoroquinolones, 3rd- and 4th-generation cephalosporins, macrolides, glycopeptides and polymyxins, as well as other antimicrobials such as antiparasitic drugs, play a significant role in antimicrobial resistance (AMR). Overuse and misuse of these compounds promote resistance, reducing the effectiveness of treatments for bacterial, parasitic, viral, and fungal infections and posing a major global health risk [1,2]. AMR is a pressing worldwide challenge, directly associated with 1.27 million deaths in 2019 [3]. Aquatic environments are particularly affected, as pharmaceuticals enter water bodies through leakage, runoff, manure application, improper disposal, and direct aquaculture release. Over 70 compounds—predominantly antibiotics—have been detected in surface waters [4], and antimicrobial use in aquaculture is projected to surpass human consumption by 80% by 2030 [5]. Residual and resistant antimicrobials can disrupt microbial diversity, alter biogeochemical cycles, and reduce biodiversity, producing cascading effects on aquatic food webs and potentially impacting human health [6].

Case studies from our laboratory further show that antibiotics and ectopesticides affect aquatic organisms across different trophic levels and developmental stages—from whole organisms down to cellular responses—even at concentrations commonly detected in aquatic environments [7,8].

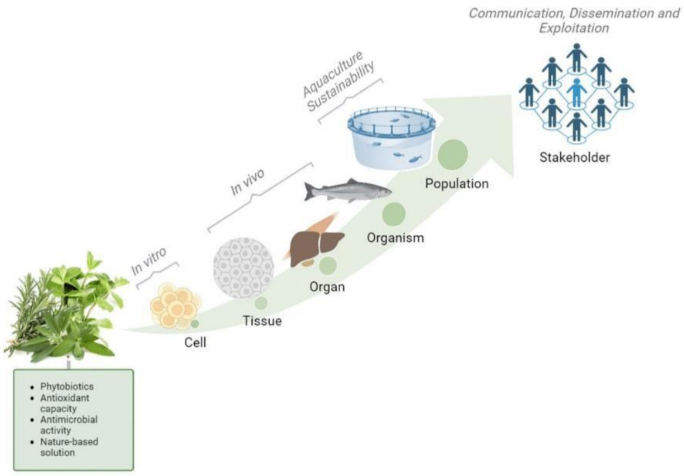

Figure 1:Graphical representation of the SOURCE project impact

Given these challenges, the unsustainable practices of certain aquaculture systems must be addressed. Developing alternative biocontrol strategies is urgently needed to ensure the sustainable management of aquaculture within the One Health framework. In this context, our multidisciplinary project *SOURCE*, funded under *Italian Fund for Science*, investigates the potential of phytobiotics as sustainable alternatives to antibiotics in aquaculture, with the overarching goal of enhancing animal health, reducing environmental impacts, and generating evidence-based guidelines and recommendations to promote One Health–aligned management practices.

[1] European Medicines Agency (EMA). Categorization of antibiotics. Eur. J. Pharm. Sci. 2023, *106473.*
[2] World Health Organization (WHO). Antimicrobial Resistance Factsheet. WHO, 2023.
[3] World Health Organization (WHO). Global burden of bacterial antimicrobial resistance, 2021.
[4] Wang, C., et al. J. Hazard. Mater. 2023, *132431.*
[5] Schar, D., et al. Sci. Rep. 2020, *10, 8274.*
[6] Cabello, F.C., et al. Rev. Aquacult. 2022, *14, 1–23.*
[7] Giannessi, J., et al. Heliyon 2024, *10, e40467*.
[8] De Marchi, L., et al. 2025, *15, 1533*.

KN4

Exploring the role of enantioselectivity in environmental processes

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Chiral compounds may have one or more chiral centre (*e.g.,* asymmetric carbon atom) in their structure, originating enantiomers that are stereoisomers which differ from each other as non-superposable mirror images [1]. The different three-dimensional molecular structures of a pair of enantiomers leads to enantioselectivity since binding-molecules have the capacity to recognize enantiomers in a different way. In fact, different biological and toxicological effects are widely recognized, with the "thalidomide tragedy" being the most remarkable and tragic example of enantioselectivity. However, the impact of the dissimilar behaviour between a pair of enantiomers is generally neglected in the environmental processes. Considering that many contaminants of emerging concern are chiral (*e.g.*, pharmaceuticals, drugs of abuse, pesticides), it is urgent to consider enantioselectivity in the context of environmental pollution and ecological impact. Therefore, understanding stereoselectivity in the environmental fate, distribution, (bio)transformation, (bio)degradation, ecotoxicity, and bioaccumulation of chiral compounds is crucial. For an accurate understanding of enantioselective processes, a combination of advanced analytical techniques, comprehensive degradation and ecotoxicological studies, and risk assessment, is needed [1]. Examples of enantioselective environmental studies will be presented and discussed.

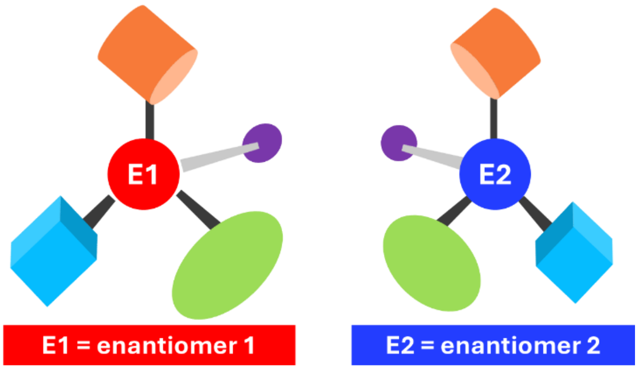

Figure 1: Representation of the three-dimensional asymmetry of the enantiomers of a chiral compound.

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[1] Ribeiro, A.R.L.; Maia, A.S.; Ribeiro, C.; Tiritan, M.E. in Mass Spectrometry in Food and Environmental Chemistry. *The Handbook of Environmental Chemistry*, 2022, *119*, Y. Picó, J. Campo (Eds.) Mass Spectrometry in Food and Environmental Chemistry, Switzerland, Springer Cham

Oral
Communications

OC1

Monitoring Endocrine-Disrupting Pharmaceuticals in Belgian Tap and Bottled Water: Insights from the AquaGlance Study

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Endocrine-disrupting compounds are increasingly linked to chronic health conditions, including hormone-related cancers, metabolic disorders, reproductive impairments, and thyroid dysfunction. Their persistence in drinking water is largely attributed to the limited efficacy of conventional wastewater treatment systems in removing pharmaceuticals at trace concentrations, underlining the importance of continuous environmental monitoring.

Within the AquaGlance study, we investigated the occurrence of endocrine-disrupting pharmaceuticals, including acetaminophen, carbamazepine, propranolol, citalopram, chlorothiazide, as well as synthetic hormones 17β-estradiol, and dexamethasone in 37 commercially bottled water brands and tap water from 300 households across diverse regions in Flanders, Belgium. A sensitive multiresidue analytical method was developed and successfully validated using solid-phase extraction coupled with ultra-high performance liquid chromatography–high resolution mass spectrometry (Orbitrap Exploris 120), achieving quantification limits between 1–5 ng/L. Analyte stability was confirmed for 72 hours under dark storage conditions.

In bottled water, acetaminophen was detected in 26 of 37 samples (C_{max} = 60.2 ng/L). Trace amounts of citalopram and triclosan (<5 ng/L) were identified in 2 and 1 out of 37 samples, respectively. In addition, dexamethasone was detected in 2 samples through suspect screening using full-scan acquisition on the high-resolution Orbitrap mass spectrometer, subsequently confirmed at a concentration of 21 and 24 ng/L. Ordinary Least Squares regression analysis indicated no statistically significant influence of bottle type, source type (spring vs. mineral), or retail price on pharmaceutical and hormonal occurrence, except for dexamethasone only occurring in glass bottled waters. Results from the ongoing tap water analysis will be presented at the conference.

Given the absence of regulatory thresholds for pharmaceuticals in drinking water, the WHO recommends maintaining concentrations as low as reasonably achievable. Future work will integrate chemical monitoring data with consumer exposure questionnaires to enable a more comprehensive, exposure-based risk assessment. In the absence of specific regulatory limits, a tiered risk assessment approach -beginning with conservative estimates and incorporating computational toxicology and animal studies - remains essential to guide public health protection.

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OC2

Water fleas as “canaries in the coal mine” for the detection of pharmaceuticals in the environment

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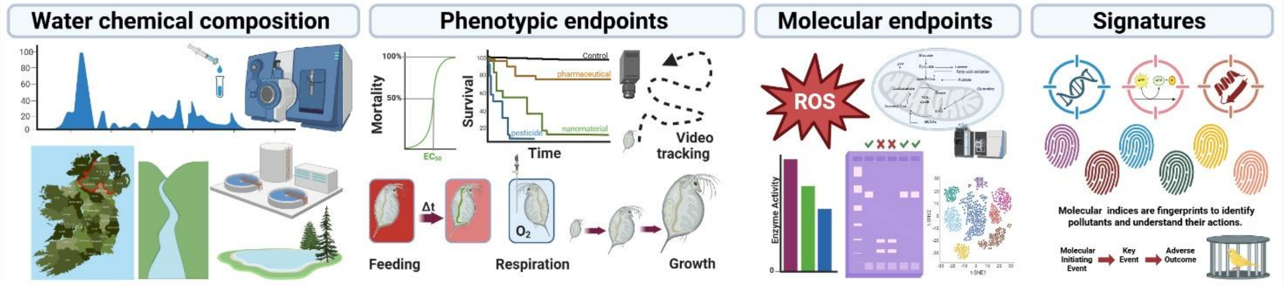
The ongoing rise in the global aging population, coupled with the excessive use of various resources, has significantly exacerbated environmental challenges, with the increased detection of pharmaceuticals in surface waters. This situation poses serious risks to aquatic ecosystems and human health. While various analytical techniques are employed in water monitoring to identify contaminants, the analytical methods employed are often inadequate for providing early predictions or for fully capturing the underlying mechanisms for the observed effects in the ecosystem. This limitation highlights the need for more comprehensive approaches to pollution assessment. Consequently, there is a growing support from effect-based methods that assess the responses of key species, such as daphnids, to pollutants. Daphnids are critical freshwater organisms that serve as valuable indicators of ecosystem health. In the context of New Approach Methodologies, they provide significant advantages due to their alignment with the principles of the 3Rs (Reduce, Refine, Replace) and their similar toxicity responses to more complex organisms, enhancing the application from phylotoxicological studies. Our research focuses on the impact of a range of commonly encountered pharmaceuticals on the physiology of daphnids. By integrating phenotypic endpoints, such as growth and reproduction, with metabolic fingerprints, we aim to provide deeper mechanistic insights into the actions of these pollutants. Ultimately, identifying metabolic disruptions can yield more sensitive assessment metrics, allowing us to capture the mechanisms of action more accurately. This enables timely predictions of pollution hotspots, facilitating proactive management strategies to mitigate environmental damage before it becomes irreversible.



OC3

Environmental quantification and fate of therapeutic modified oligonucleotides in mixed liquor suspended solids

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Increasingly, modified oligonucleotides (mONs) are being introduced as biochemicals, with applications in the pesticide and pharmaceutical industries [1-2]. mONs function via various gene silencing mechanisms including mRNA degradation, steric hindrance, splicing modulation, and protein inhibition [3], with chemical modifications (e.g., phosphorothioate backbone bonds, methylation of backbone sugars) aiding delivery and performance [1]. Evidence suggests that mONs potentially threaten ecosystem and human health in the environment similarly to other pharmaceutical modalities [4]. Furthermore, mONs may hybridize to non-target sequences, leading to unintentional gene silencing in the environment [5]. While mONs have been studied in multiple environmental matrices [6-7], the fate and transport of therapeutic mONs are understudied in wastewater. As a proof of concept, two modifications (methoxyethyl group addition to the backbone adenines and phosphorothioate bonding) were introduced to the DNA reverse transcript of a Bovine Coronavirus (BCoV) sequence and spiked into mixed liquor suspended solids (MLSS) collected from the Boulder Water Resource Recovery Facility in Boulder, Colorado, USA. To observe the degradation of the mONs, five temporal samples were taken over a 24-hour period. Raw MLSS and autoclaved MLSS experimental conditions facilitated differentiation between biotransformation and other reactions or partitioning processes. While mONs can be detected and quantified through quantitative polymerase chain reaction (qPCR), the replication process is disrupted by the addition of chemical modifications. This study adapts and optimizes an existing qPCR method for the quantification of mONs [8], including the BCoV sequence and therapeutic mON sequences approved for medical use. Preliminary results indicate that biotransformation is a main degradation mechanism for the modified BCoV sequence, and additional experiments will observe the degradation of other mONs and therapeutic mONs in MLSS. Additionally, the fate and transport of mONs in municipal wastewater systems are modeled by the authors' app, SeweRx, which predicts the concentrations of various pharmaceuticals in wastewater influent from data on pharmaceutical consumption, community demographics, and in-sewer hydrolysis, biotransformation, and sorption processes. The SeweRx simulation and bench-scale experiments together provide a more complete understanding of the fate of therapeutic mONs in wastewater systems.

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[1] Vinjamuri, B. P.; Pan, J.; Peng, P.A. *J. Pharm. Sci.* 2024, *113*, 1749-1768. [2] Gal'chinsky, N.V. et al. *Pestic. Biochem. Physiol.* 2024, *200*, 105838. [3] Kilanowska A.; Studzińska, S. *RSC Adv*. 2020, *10*, 34501-34516. [4] Un Jan Contreras, S. et al. *Environ. Sci. Technol*. 2024, *53*, 13856-13865. [5] Jung, J. et al. *RNA*. 2023, *29*, 570-583. [6] Bachman, P. et al. *Front. Plant Sci*. 2020, *11,* 21. [7] Parker, K.M. ; Sander, M. *Environ. Sci. Technol.* 2017, *51,* 12049-12057. [8] Shin, M. et al. *Nucleic Acid Ther*. 2022, *32,* 66-73.

OC4

Lessons Learned from Two Decades of Research on Uncovering Emerging Contaminants and Their Ecological Impacts

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In the last twenty years, thousands of research papers covering different aspects of emerging contaminants have been published, ranging from environmental occurrence to treatment and ecological effects. Emerging contaminants are environmental pollutants that have been investigated only in the last 20 years, and include man-made and naturally occurring chemicals such as pharmaceuticals, personal care products, illicit drugs, engineered nanomaterials, and antibiotic resistance genes. The advancement in our knowledge on emerging contaminants has been driven by the introduction of highly sensitive and powerful analytical instrumentation that allowed trace quantification and identification of contaminants in complex environmental matrices. High efficiency chromatographic separations couples to high-resolution mass spectrometers have become commonplace in environmental laboratories, increasing our understanding and awareness of the presence of emerging contaminants in the environment, their transformation and fate, and the complex ecological consequences that they pose on biological systems. In this presentation an overview on important research milestones in the area of emerging contaminants, focusing on the fate and treatment of pharmaceuticals and endocrine disrupting compounds in municipal and agricultural wastewater, will be presented. In addition, novel applications of mass spectrometry to assess occurrence and effects of emerging contaminants at sub-lethal concentrations will be discussed.

OC5

Fabrication of an electrochemical sensor based on nanoclusters with carbon nanotubes for the determination of ethylmorphine

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The opioid analgesic and antitussive drug ethylmorphine (EM) is used to treat pain and lessen coughing. Despite its widespread usage as a painkiller, opioids lead to addiction, overuse, and overdose deaths. Because of worldwide risks, pharmaceutical environmental contamination has gained international attention. Therefore, it is necessary to develop reliable, fast, and sensitive analytical tools to determine EM.

This work developed a novel electrochemical sensor based on Cu/Au bimetallic nanoclusters (NCs) and multi-walled carbon nanotubes (MWCNTs) to detect EM. Firstly, Cu/Au bimetallic nanoclusters were synthesized with some changes [1]. The synthesized nanocluster was characterized by X-ray photoelectron spectroscopy (XPS), and the binding energies of Au 4f7/2 and 4f5/2 are 84 eV and 88 eV, respectively. The binding energies of Cu 2p are 932 eV and 952 eV, consistent with literature reports. Then, modification with layer by layer (5 µL x 3 layer) of MWCNTs, NCs, and MWCNTs@NCs increases the peak current of EM by almost 30, 3, and 52 times higher than the bare electrode, respectively. The mechanism of ethyl morphine was investigated in the supporting electrolytes such as acetate (pH 3.6, 4.7, and 5.1), phosphate (pH 1.7, 2.0, and 3.0), and Britton Robinson buffers in the pH range between 2.00 and 9.00 with the bare glassy carbon electrode. The highest peak current of EM was obtained in the phosphate (pH 3.0) and acetate (pH 4.7) buffer solutions. The voltammetric studies were conducted at various scan rates ranging from 5 to 750 mV/s with these two buffer solutions. In the phosphate (pH 3.0) buffer solution, the slope of the log of peak current as a function of the log of scan rate is 0.34, so a diffusion-controlled mechanism controls the electron transfer. There are ongoing studies about the analytical performance of the sensor. The designed electrochemical sensor was developed based on the unique electronic properties of NCs, the high surface area of MWCNTs, and their combined synergistic effect.

[1] Kong, L.; Chu, C.; Wang, H.; Zhou, Y.; Liu, W. *Nanoscale* 2018, *10*, 1631.

OC6

Nanomaterials-Supported MIP-Based Electrochemical Sensor for the Determination of Lenalidomide: Application to Environmental Matrices

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Lenalidomide (LEN) is a potent immunomodulatory medication commonly used to treat multiple myeloma and other hematologic malignancies due to its ability to suppress tumor growth and modulate immune system response [1].

Developing a nanomaterial-supported molecularly imprinted polymer (MIP)-based electrochemical sensor enabled the sensitive and selective determination. The sensor was established via photopolymerization (PP) on a glassy carbon electrode (GCE) utilizing LEN as the template and 3-aminophenylboronic acid (3-APBA) as the functional monomer. Cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and scanning electron microscopy (SEM) were used to characterize the MIP-based electrochemical sensor. Differential pulse voltammetry (DPV) with 5.0 mM $[Fe(CN)_6]^{3-/4-}$ as the redox probe was employed for LEN detection in standard solutions, biological serum, and tap water samples. Following optimized experimental conditions, the dynamic linear range of the performed sensor was found to be 1.75×10^{-12} to 2.5×10^{-11} M for the DPV method. The limits of detection (LOD) and quantification (LOQ) were determined to be 0.42 pM and 1.40 pM, respectively. The fabricated sensor demonstrated excellent detection ability for LEN in the presence of its analogs, as well as other interfering solutions. In conclusion, the presented sensor showed good selectivity and high sensitivity for LEN determination in biological serum and tap water samples, demonstrating its applicability for both biological and environmental analysis.

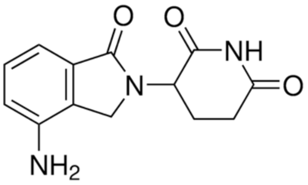

Figure 1. *Molecular Structure of LEN*

Acknowledgments: The author would like to thank the Embassy of Libya, Academic Attaché Office, Ankara/ TÜRKİYE, for supplying financial support with Scholarship number 1359.

[1] Kulig P, Milczarek S, Bakinowska E, Szalewska L, Baumert B, Machaliński B. Cancers. 2023;15(3):9

OC7

From powder to beads: synthesis and shaping of an imine-linked triazine porous organic polymer for antibiotic remediation from water

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Water pollution, particularly with antibiotics, contributes to the induction and spread of antimicrobial resistance, which are two of the main problems plaguing humanity [1,2,3]. To address these issues, effective yet straightforward remediation strategies are urgently needed [4]. This communication describes an imine-linked triazine porous organic polymer (IT-POP, Fig. 1A) as a novel highly stable micrometer-sized advanced adsorbent, featuring hydroxyl and carboxyl functional groups (0.43 mmol g^{-1}). Upon deprotonation of its carboxyl groups, IT-POP acquires a negative surface charge (isoelectric point at pH = 4.7), which promotes the efficient adsorption of ciprofloxacin (CPX) and levofloxacin (LVX) antibiotics, with removal efficiencies up to 99% (Fig.1B) and maximum sorption capacities up to 0.34 mmol g^{-1}. To facilitate practical application, IT-POP was incorporated into starch-alginate beads. Beads containing 10 w/w% of IT-POP (Fig. 1C) showed excellent performance, offering an economical and scalable solution for day-to-day application. Remarkably, even with a 10-fold reduction in the content of IT-POP functional material, the adsorption capacities of CPX and LVX decreased only 2-fold, representing a 5× enhancement in the performance of IT-POP after its incorporation into the polysaccharide matrix. The powder material and the composite beads effectively removed 6 out of 7 tested antibiotics at micromolar concentrations, showing residual affinity for amoxicillin and greater selectivity for sulfonamides (sulfadiazine, sulfamerazine, sulfamethazine), tetracycline, and fluoroquinolones (CPX and LVX). The materials also exhibited high reusability over 5 cycles and maintained good removal performance in wastewater samples, confirming their applicability in real environmental conditions. Furthermore, comparative studies between batch and continuous flow systems reaffirmed the strong potential of the proposed adsorbents for the decontamination of antibiotic-containing effluents.

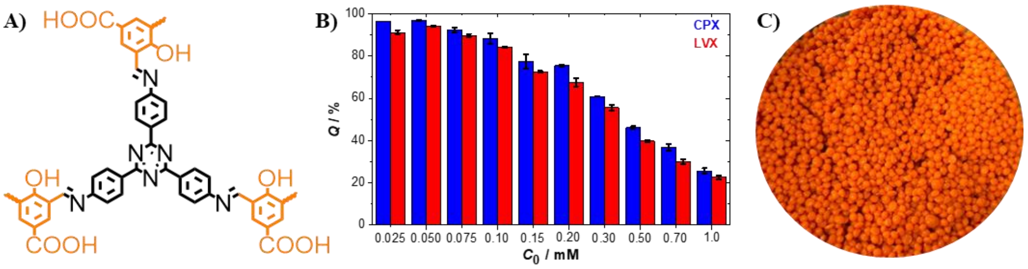

Figure 1: A) Chemical structure of IT-POP; B) Effect of the initial concentration on the removal efficiencies of CPX and LVX by IT-POP; C) Photograph of IT-POP-containing starch-alginate beads.

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[1] Gaur, N.; Sharma, S.; Yadav, N. Environmental Pollution. In *Green Chemistry Approaches to Environmental Sustainability*; Elsevier, 2024; pp 23–41.
[2] Matias, P. M. C.; B. Rodrigues, A. C.; Nunes, S. C. C.; Canelas Pais, A. A. C.; Murtinho, D.; Valente, A. J. M. *Environmental Pollution* 2024, *363*, 125197.
[3] Matias, P. M. C.; Nunes, S. C. C.; Rodrigues, A. C. B.; Ltayef, M.; Sellaoui, L.; Mbarek, M.; Murtinho, D.; Canelas Pais, A. A. C.; Valente, A. J. M. *Sep Purif Technol* 2025, *355*, 129731.
[4] Song, W.; Zhang, Y.; Tran, C. H.; Choi, H. K.; Yu, D.-G.; Kim, I. *Prog Polym Sci* 2023, *142*, 101691.

OC8

The Investigation of Simultaneous Nitrate and Pharmaceuticals Removal from Wastewater Treatment Plant Effluents through Sulfur-Based Autotrophic Denitrification Processes

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This study investigates the co-removal efficiency of nitrate and five widely used pharmaceutical compounds - triclosan, ibuprofen, carbamazepine, naproxen, and diclofenac in a lab-scale autotrophic denitrification column bioreactor. Nitrate concentrations (5–30 mg/L) and pharmaceuticals (constant at 5 µg/L) will simulate domestic wastewater effluent. The study evaluates the effect of nitrate concentration on pharmaceutical removal and the potential impact of pharmaceuticals compounds on the denitrification process.

Nitrates frequently co-occur with pharmaceutical active compounds (PhACs) in domestic and industrial wastewaters [1], making their simultaneous removal an environmentally relevant challenge.

A lab-scale sulfur-based autotrophic denitrification bioreactor (150 mL total, 75 mL bed volume) was operated continuously in up-flow mode at room temperature. The reactor, filled with elemental sulfur, serving as both electron donor and biofilm carrier, was inoculated with sludge from a municipal wastewater treatment plant (WWTP).

During the acclimation phase, a nitrogen loading rate of 170 mg N/L/day with a 15-hour hydraulic retention time (HRT) for the first 15 days. This was subsequently reduced to 100 mg N/L/day and 8-hour HRT to simulate steady-stable operation. The reactor achieved an average nitrate removal efficiency of 93%, indicating successful microbial acclimation (Figure 2). Effluent sulfate concentrations were positively correlated with nitrate removal, as shown by measured and theoretical sulfate concentrations.

Post-acclimation, influent nitrate concentrations will be varied between 5 and 30 mg/L while maintaining constant nitrate loading by adjusting HRT.

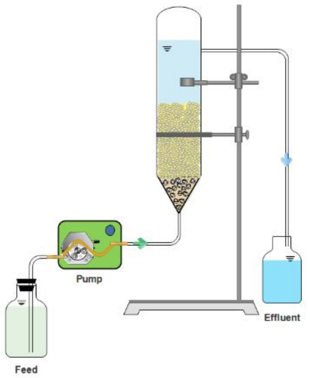

Figure 1: Schematic view of reactor

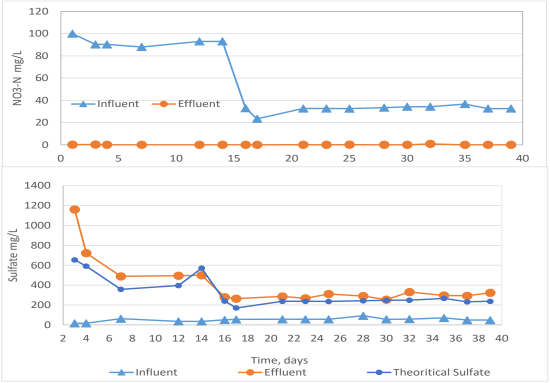

Figure 2 : Variation of nitrate and sulfate concentration in acclimation period

Pharmaceutical concentrations in the effluent will be evaluated using liquid chromatography-mass spectrometry (LC-MS).

Acknowledgements: This study was supported by the Scientific and Technological Research Council of Türkiye (TÜBİTAK) under the 2219 International Postdoctoral Research Fellowship Program and by the University of Basilicata.

[1] W. Zhu, Z. Tang, G. Peng, Z. Wang, W. Wang, Y. Zhang, J. Wang, S. Zhang, J Clean Prod (2024) 434.

OC9

Efficient Removal of 17α-Ethinylestradiol from Water Using Silica-Based Adsorbents: Impact of Organic Functionalities and Water Matrices

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Three silica-based porous adsorbents – MCM-41 (pure silica), vinyl-MCM-41 (hybrid silica), and Ph-PMO (periodic mesoporous phenylene-silica) – were tested to evaluate the effect of organic functionalities on removing the hormone disruptor 17α-ethinylestradiol (EE2) from water. Adsorbent dosages were tested in ultrapure water spiked with 200 $\mu g\ L^{-1}$ of EE2, and the results revealed that concentrations higher than 500 $mg\ L^{-1}$ of adsorbent did not significantly enhance the EE2 removal efficiency. Both materials containing organic functionalities (using a dose of 500 $mg\ L^{-1}$) were tested in ultrapure water, phosphate buffer at pH 5, 7, and 9, and wastewater effluent to evaluate the pH impact and effect of different water matrices on their adsorption performance. An increase in pH significantly improved the EE2 adsorption capacity of Ph-PMO, reaching 94 ± 2 % at pH 9, while it decreased the adsorption efficiency of vinyl-MCM-41 to 14 ± 7 % at the same pH. Following a comprehensive characterization of the materials, including assessments of chemical stability across varying pH conditions, point of zero charge, hydrophobicity, and textural properties such as specific surface area, pore volume, and pore diameter, the findings suggests that the homogenous distribution of organic functionalities in Ph-PMO enhances surface interactions, such as π-π stacking and hydrophobic interactions, with the EE2 hormone. Ph-PMO demonstrated superior performance in wastewater effluents, and kinetic studies showed rapid EE2 adsorption across all matrices, reaching equilibrium within 5 minutes. This study highlights the suitability of Ph-PMO for water remediation applications.

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OC10

Removal of venlafaxine from water through carbon adsorbents produced from spent brewery grains

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The high human consumption of the antidepressant drug venlafaxine (VFX) has increased in recent years due to the rise in depression cases [1]. The incomplete removal of this antidepressant in wastewater treatment plants (WWTPs) has led to its growing presence in aquatic environments. VFX is now recognized as an emerging contaminant (EC), posing adverse toxicological effects to both the environment and human health [2]. Consequently, it was included in the 2022 Watch List of Substances by the European Commission (Decision 2022/1307/EC). Generally, ECs are highly stable compounds that are difficult to degrade or remove effectively using conventional WWTP treatments. This persistence results in their discharge in effluents, re-entering rivers and lakes, and negatively impacting humans and ecosystems. Thus, implementing efficient treatments to remove ECs before effluent discharge is crucial.

In this context, adsorptive treatments have gained renewed attention in recent years due to their effectiveness in removing these recalcitrant contaminants without by-product formation [3]. Carbon materials, namely activated carbons (ACs), have been widely used as efficient adsorbents due to their large specific surface area (S_{BET}), high porosity, favorable pore size distribution, and potential for surface functionalization [3]. The adsorption performance and cost of ACs depend on factors such as the activation method, precursor material, and thermal treatment. To align with circular economy principles, agricultural and industrial wastes have been explored as sustainable AC precursors, as a way to valorize these underused sources of carbon. In this study, spent brewery grains (SBG), a lignocellulosic waste comprising about 85% of the brewing industry's total waste, were used as the precursor for AC production [4]. Potassium carbonate (K_2CO_3) was used as the activating reagent during AC synthesis. The impregnated raw material then underwent two types of pyrolysis: conventional and microwave-assisted. This approach aimed to evaluate the impact of different thermal treatments on the adsorptive properties of the resulting materials. Microwave-assisted pyrolysis offers a strategic advantage, overcoming the limitations of conventional methods by providing rapid and uniform heating, which results in shorter production times and lower energy consumption [5].

For practical applications, evaluating AC performance under conditions as realistic as possible is critical. This involves assessing matrix and competitive effects on VFX removal in effluents from WWTPs. Therefore, the adsorption kinetics, equilibrium isotherms, and adsorption capacity of AC-SBG towards VFX were determined in biologically treated urban wastewater. Comparing the two ACs, the one obtained by microwave pyrolysis showed superior performance, with adsorption equilibrium reached in only 2 hours and VFX removal efficiencies of 61.2% and 58.5% (with an AC dose of only 50 mg/L) in ultrapure and wastewater, respectively.

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[1] Valenzuela, L.; Pedrosa, M.; Bahamonde, A.; Rosal, R.; Torres-Pinto, A.; Silva, C. G.; Faria, J. L.; Silva, A. M. T. *Catal. Today* 2023, vol. 418.
[2] Cerrato-Alvarez, M.; Rioboó-Legaspi, P.; Costa-Rama, E.; Fernández-Abedul, M. T. *Biosens. Bioelectron.* 2025, vol. 267.
[3] Ahmed, M. J. *J. Environ. Manage.* 2017, vol. 190, pp. 274–282.
[4] Sousa, A. F. C.; Gil, M. V.; Calisto, V. *Environ. Sci. Pollut. Res.* 2020, vol. 27, pp. 36463–36475.
[5] Sousa, É.; Rocha, L.; Jaria, G.; Gil, M. V.; Otero, M.; Esteves, V. I.; Calisto, V. *Sci. Total Environ.* 2021, vol. 752, p. 141662.

OC11

Effect of diclofenac on wastewater treatment with aerobic granular sludge: performance and biopolymer production

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Diclofenac (DCF) is an anti-inflammatory drug regarded as a contaminant of emerging concern due to its extensive use and resistance to removal in wastewater (WW) treatment plants. Aerobic granular sludge (AGS) technology, known for its excellent settling capacity, resilience against perturbations, and nutrient removal efficiency, shows promise in WW treatment. This work aimed to determine AGS's potential to tolerate DCF at environmentally relevant concentrations (up to 70 µg L^{-1}) and assess its effect on AGS carbon and nutrient removal and on the production of biopolymers (i.e. polyhydroxyalkanoates (PHAs) and glycogen).

The experimental system consisted of a 2-L anaerobic-aerobic sequencing batch reactor (SBR) inoculated with AGS from a Municipal Wastewater Treatment Plant (Frielas, Loures, Portugal). The SBR was operated in 6h-cycles with 12h of hydraulic retention time, 50% volumetric exchange ratio, and no imposed solids retention time. Each cycle had 1h of non-aerated reaction followed by 4h of aeration. Synthetic WW comprising acetate, ammonium, phosphate, and micronutrients in addition to DCF, was prepared with a C:N:P ratio of 100:7:1, according to Table 1.

Table 1: SBR experimental periods.

Acetate concentration in Synthetic WW ($mgO_2\ L^{-1}$ as COD)	OLR ($gCODL^{-1}d^{-1}$)	Diclofenac concentrations in Synthetic WW (µg L^{-1})
800	6.4	0;40;70
1600	12.8	0;40;70
3200	25.6	0;40;70

In general, DCF appeared not to impact directly the total carbon source removal, since complete acetate uptake was observed at the end of every cycle. Nonetheless, the higher the C-source concentration, the longer the AGS took to consume it, regardless of the DCF concentration. For organic loading rate (OLR) values of 6.4 and 12.8 $gCODL^{-1}d^{-1}$, acetate was totally consumed at the end of the non-aerated reaction stage, and for 25.6 $gCODL^{-1}d^{-1}$, total acetate removal only occurred after the first hour of the aerated stage. Ammonium removal profiles remained similar, independently of the DCF concentration, but enhanced biological phosphorus removal by polyphosphate accumulating organisms (PAO) was negatively affected by DCF. Also, regardless of the C-source concentration, the presence of DCF inhibited glycogen accumulating organisms (GAO) activity, since the increase in DCF concentration resulted in a decrease of the stored glycogen concentration (Figure 1). The opposite behavior was observed for PHA, as the highest intracellular PHA content values were attained when AGS was exposed to the highest DCF concentration (Figure 1). Regarding AGS physical robustness, the granules' settle ability was not affected by either DCF or C,N,P concentrations.

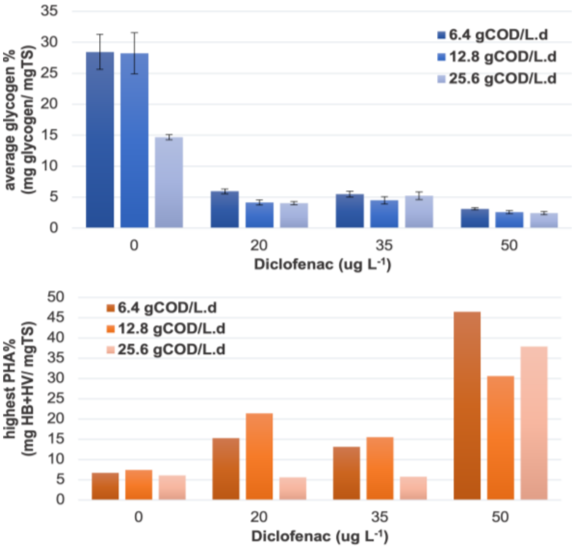

Figure 1: Effect of DCF concentration on glycogen and PHA content (%m/m).

Exposure to DCF decreased AGS solid content: the higher the DCF content, the bigger the impact.

The presence of DCF in environmental relevant concentrations appears to negatively impact PAO and GAO metabolism and to induce PHA production.

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OC12

Sustainable Fixed-Bed Adsorption of Antibiotics from Wastewater Using Regenerable Biochar Derived from Brewery Residues

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The increasing occurrence of antibiotics in aquatic environments poses critical environmental and public health challenges due to their contribution to antimicrobial resistance. In response, the revised European Urban Wastewater Treatment Directive has introduced stricter requirements for the implementation of advanced treatments in wastewater treatment plants (WWTPs), emphasizing the urgent need for cost-effective and sustainable remediation technologies [1]. In this context, the valorization of agro-industrial residues as precursors for producing efficient adsorbents to remove antibiotics from wastewater represents a promising strategy. Among these residues, spent brewery grains (SBG), stand out as an abundant, low-cost, and renewable precursor for biochar (BC) production, supporting circular economy principles while addressing environmental sustainability.

This work investigates the performance of BC produced from SBG for the fixed-bed adsorption of three widely detected antibiotics (sulfamethoxazole (SMX), trimethoprim (TMP), and ciprofloxacin (CIP)) from water. The influence of flow rate, aqueous matrix, and single *vs.* multi-component systems on the breakthrough adsorption behavior was systematically evaluated. Furthermore, the thermal regeneration of the exhausted BC and its reuse in subsequent adsorption cycles were assessed. A life cycle assessment (LCA) evaluated environmental performance, identifying key impact stages and optimization opportunities.

BC was produced via microwave-assisted pyrolysis (800 °C during 20 min). Fixed-bed experiments were conducted using a jacketed column (13 cm length, 1 cm inner diameter) packed with 2.0 g of BC at a bed depth of 4.4 cm and operated at 25 ± 1 °C. The study was performed in three stages: (i) optimization of flow rate (1, 2, and 4 $L\ d^{-1}$) using buffered distilled water at pH 8.0; (ii) evaluation of adsorption from single and ternary antibiotic solutions at the optimal flow rate (2 $L\ d^{-1}$); and (iii) thermal regeneration of the exhausted BC via microwave pyrolysis (600 °C, 20 min) and testing over two additional adsorption cycles using TMP as a case study. Breakthrough data were fitted to the Thomas, Yan, and Yoon–Nelson models. Among the antibiotics, BC exhibited the highest bed adsorption capacity for TMP, followed by CIP and then SMX, likely due to electrostatic repulsion between SMX and BC at pH 8. In ternary solutions, adsorption capacities decreased compared to single-component systems, suggesting competitive effects. Thermal regeneration significantly enhanced BC performance, increasing S_{BET} from 281 $m^2\ g^{-1}$ in cycle 1 to 462 $m^2\ g^{-1}$ in cycle 3. LCA showed that the major contributors to the environmental impacts were the chemicals and electricity consumed in the laboratory drying stage of the BC-SBG precursor, and the combustion flue gases emitted from pyrolysis vapors combustion. This study highlights the potential of SBG-derived BC as a sustainable, regenerable adsorbent for pharmaceutical removal in continuous fixed-bed systems.

Acknowledgements:
This work was developed within the project SYNERGY (2022.02028.PTDC, doi.org/10.54499/2022.02028.PTDC), supported by national funds (OE), through FCT/MCTES. The authors also acknowledge financial support to CESAM by FCT, under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020).

[1] European Comission, Proposal for a Revised Urban Wastewater Treatment Directive-European Commission 2024.

OC13

Efficiency of the Asian Clam in Removing Pharmaceuticals from Wastewater.

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Human excretion is the primary source of pharmaceutical residues in the aquatic environment, with wastewater treatment plants (WWTPs) acting as major pathways for the dissemination of these contaminants. Incomplete removal during conventional treatment processes facilitates the release of pharmaceuticals and their metabolites into surface and marine waters, thereby increasing exposure risks for aquatic organisms and potentially impacting ecosystem health [1,2].

Given that WWTPs are not fully effective at eliminating pharmaceutical compounds, a tertiary (polishing) treatment process was assessed using the freshwater bivalve *Corbicula fluminea*. This experimental study was conducted within the framework of the BIOFREE project.

The methodology involved the use of wastewater, *C. fluminea* specimens, and appropriate containment systems for controlled exposure. Key experimental parameters included exposure time, reusability of the clams, and their removal efficiency. A 20 L effluent sample was collected from Choupal WWTP (Coimbra), and clams (*C. fluminea*), from Central Portugal, were depurated in clean water for 7–10 days to eliminate pre-existing contaminants before use. The clams were exposed to the effluent wastewater for 24 and 48 hours. The procedure was then repeated using the same clams, following a depuration period, in order to evaluate their performance upon reuse under the same exposure conditions. A blank control assay was also conducted using only the effluent water from the WWTP and the aeration system, in the absence of clams. Water samples were analysed for 19 pharmaceuticals belonging to different therapeutic groups by solid phase extraction (SPE) following ultra-high performance liquid chromatography coupled with time-of-flight mass spectrometry (UHPLC-ToF-MS).

Out of the 19 pharmaceuticals investigated, 13 were effectively removed by the clams, both in their initial use and after reuse. The results showed an average removal of 36.6% with statistically significant removal efficiencies, particularly for antihypertensive agents (48.3%), neuroactive pharmaceuticals (42.9%), and antibiotics (35.0%). No significant differences were observed between exposure of 24 hours (36.7–37.8%) and 48 hours (38.7–44.7%), indicating that extended exposure may not substantially enhance performance. Additionally, reuse of *C. fluminea* yielded comparable removal rates, suggesting the potential for operational sustainability.

This study highlights the potential of a novel, nature-based polishing treatment for the removal of pharmaceutical contaminants from wastewater. The approach is both promising and practical, offering a sustainable, low-cost solution suitable for implementation in WWTPs, particularly in resource-limited or underdeveloped regions. Furthermore, it promotes the valorisation of an invasive species through its removal from natural ecosystems and integration into an environmentally beneficial application.

Acknowledgements: This research was funded by FCT/MCTES (UIDB/50006/2025 | REQUIMTE | LAQ.V) through national funds. The authors also acknowledge the BIOFREE UC/SANTANDER project

[1] Pereira, A.M.P.T.; Silva, L.J.G.; Laranjeiro, C.S.M.; Meisel, L.M.; Lino, C.M.; Pena, A. Human Pharmaceuticals in Portuguese Rivers: The Impact of Water Scarcity in the Environmental Risk. *Sci. Total Environ.* 2017, *609*, doi:10.1016/j.scitotenv.2017.07.200.

[2] Rodrigues, F.; Durães, L.; Simões, N.E.C.; Pereira, A.M.P.T.; Silva, L.J.G.; João Feio, M. Pharmaceuticals in Urban Streams: A Review of Their Detection and Effects in the Ecosystem. *Water Res.* 2025, *268*, doi:10.1016/j.watres.2024.122657.

OC14

Titanium Dioxide Nanoparticles-Integrated with MIP for Highly Selective Electrochemical Cefepime Sensing in Environmental Samples

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The broad-spectrum beta-lactam antibiotic cefepime (CFP), which belongs to the cephalosporin subgroup, is frequently used in clinical practice to treat various infections, including bacteremia, pneumonia, soft-tissue infections, febrile neutropenia, urinary tract infections, and abdominal infections [1].

In this work, we used a glassy carbon electrode (GCE) to create a MIP-based electrochemical sensor that has exceptional sensitivity and selectivity, even at trace levels. The sensor was designed by photopolymerization (PP) with CFP as the template molecule, 2-thienylboronic acid (2-TBA) as the functional monomer, ethylene glycol dimethacrylate (EGDMA) as the crosslinker, 2-hydroxymethyl methacrylate (HEMA) as the basic monomer, and 2-hydroxy-2-methylpropiophenone as the photo-initiator. To enhance the sensor's functionality, titanium dioxide nanoparticles (TiO_2NPs) were incorporated into the polymer. Furthermore, one of the most critical aspects of the sensor's design—the optimisation parameters—was optimized. Under ideal circumstances, the sensor demonstrated exceptional sensitivity and selectivity to CFP, with a linear quantification range of 10 pM to 100 pM. Tested in complex matrices, including soil and tap water samples, the sensor showed promise for dependable safety and environmental applications. Electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), scanning electron microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), and Energy-dispersive X-ray spectroscopy (EDX) were used to characterize the surface morphology and electrochemical processes. The CFP/TiO_2NPs/2-TBA@MIP-GCE sensor demonstrated effective and selective detection of CFP, even in the presence of structurally similar compounds. Moreover, its accuracy was validated by analyzing CFP spiked into soil and tap water samples.

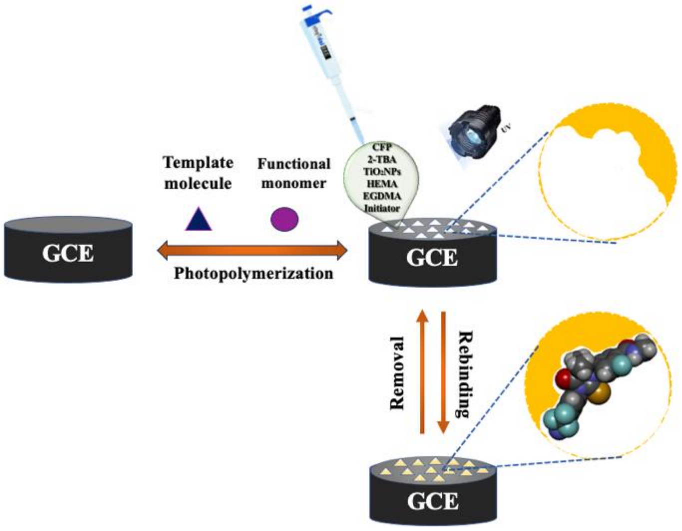

Figure 1. *Schematic representation of the developed sensor*

[1] Burgess S.V., Mabasa V.H., Bakinowska E, Chow I., Ensom M.H. 20215; 49 (3): 311-32

OC15

Assessment of the ecotoxicological effects of levamisole, an antiparasitic drug used off-label in aquaculture

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The off-label use of pharmaceuticals in aquaculture can lead to serious environmental and economic consequences. This practice involves administering drugs using treatments, dosages, or routes not authorized or regulated. Levamisole, a widely used anthelmintic in veterinary medicine, has been employed off-label in aquaculture for antiparasitic treatment in fish. This study assessed the ecotoxicological effects of Levamisole on non-target aquatic species, focusing on both acute and chronic impacts on *Daphnia similis*. Cladoceran cultivation, as well as acute and chronic toxicity tests, followed the protocols outlined in NBR 12713 [1] and OECD 211 [2]. In five acute tests, seven concentrations of Ripercol® (a commercial product containing 18.8% levamisole phosphate) were tested, ranging from 0 to 200 mg/L of Levamisole. After 48 hours of exposure, organism mobility was compared to that of a negative control group (MS medium). For the chronic test, animals at four sublethal concentrations (0 to 6.25 mg Levamisole/L) were evaluated over 21 days, monitoring reproductive output, mobility, and survival. The acute tests yielded the following mean concentrations required to cause immobility in 20%, 50%, and 80% of the organisms after 48 hours of exposure: 49.91 ± 13.80 mg/L (EC_{10}), 83.94 ± 21.09 mg/L (EC_{50}), and 141.44 ± 31.94 mg/L (EC_{80}). Significant sublethal effects were observed at 12.5 mg Levamisole/L, where exposed organisms exhibited altered movement patterns, including lethargy and erratic swimming. As concentrations increased, organisms displayed pronounced reductions in mobility and more severe behavioral changes, particularly from 100 mg/L onward. In the chronic toxicity test, lower concentrations (e.g., 0.7 mg Levamisole/L) did not produce observable effects over 21 days (NOEC – No Observed Effect Concentration). However, at higher concentrations such as 6.25 mg/L, sublethal effects including lethargy, immobility, reproductive delay, and instability were observed. Even at 2.06 mg/L (LOEC – Lowest Observed Effect Concentration), Levamisole demonstrated the potential to compromise *D. similis* survival, causing mortality on the 12th day (Figure 1).

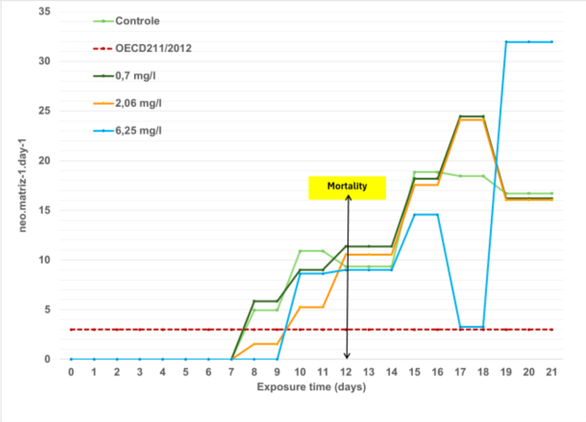

Figure 1: 21 days reproductive performance of *D. similis* exposed to Levamisole

The limited ecotoxicological data available for Levamisole primarily focus on acute tests involving *Rotifera* (*Brachionus calyciflorus*), *Chordata* (*Oryzias latipes*, *Mugil liza*), and *D. magna*. Our novel chronic toxicity findings using *D. similis* represent the most restrictive data currently available. Given the ecological importance of cladocerans in aquatic food webs, these deleterious effects raise concerns about potential disruptions to ecosystem balance. These findings highlight the need for careful monitoring and regulation of off-label antiparasitic use in aquaculture to ensure environmental sustainability.

Acknowledgements: Ministerio de Ciencia e Innovación - Agencia Estatal de Investigación (PDC 2022-133805-100)

[1] ABNT NBR 12713, Ecotoxicologia Aquática – Toxicidade aguda - ensaio com *Daphnia spp*., 2022, 31p.
[2] OECD, Test Guideline No. 211. *Daphnia magna* reproduction test. 2012, 26p.

OC16

The Effects of Ciprofloxacin on Red Sea Sponge *Stylissa carteri*: Implications of Antibiotic Pollution from Aquaculture

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Aquaculture is a source of food and income for millions of people and is a rapidly expanding industry worldwide. In Saudi Arabia, national targets aim to increase aquaculture production from 120,000 to 600,000 tons annually by 2030. While aquaculture offers promise for addressing food security, it can introduce pollutants such as excess nutrients, organic matter and chemicals [1]. One such chemical is ciprofloxacin, a broad-spectrum fluoroquinolone antibiotic used in human and veterinary medicine [2] and frequently detected in wastewater effluents due to its low biodegradability [3]. A global review reported ciprofloxacin concentrations as high as 20,321 ng/L in sewage (Gran Canaria, Spain), 6,900 ng/L in wastewater (Brisbane, Australia), and 1,300 ng/L in surface water (Kenya) [4]. Its widespread presence raises concerns about bioaccumulation and antibiotic resistance, a growing global health crisis linked to an estimated 700,000 deaths each year [5].

Ciprofloxacin has been shown to elicit sublethal physiological responses in a range of marine organisms. In vertebrates like *Danio rerio*, it alters oxidative stress biomarkers and detoxification pathways [6]; in invertebrates such as *Daphnia magna*, it induces oxidative and genotoxic damage [7]. In microalgae *Raphidocelis subcapitata* [8] and *Thalassiosira weissflogii* [9], ciprofloxacin reduces growth performance, impairs photosynthetic efficiency and increases cellular stress. These effects suggest ciprofloxacin can impact multiple trophic levels and compromise primary productivity in marine systems.

Ciprofloxacin bioaccumulation has also been documented in the marine environment. A preliminary study in the central Saudi Arabian Red Sea detected concentrations ranging from 0.45ng/L to 0.64ng/L in surface waters and 4.77ng/g to 112.11ng/g in coral tissue. Building on these findings, the present study examined the effects of ciprofloxacin on the common Red Sea sponge *Stylissa carteri* in a 14-day manipulative laboratory experiment. Exposure concentrations (50.0 ng/L, 150.0 ng/L and 450.0 ng/L) reflected both local and global environmental levels. Key physiological endpoints—including bioaccumulation, clearance rate, respiration rate, oxidative stress biomarkers, total lipid content, chlorophyll-a reflectance (as a proxy for chlorophyll-a content), and photosynthetic efficiency—were measured, alongside visual observations such as oscula closure, mucus production, tissue regression, and color change. These results will advance understanding of the environmental risks of aquaculture-derived antibiotics and provide insight into the potential of marine sponges as bioindicators and bioremediation agents for ciprofloxacin detection and removal.

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[1] Hozumi, A.; Hong, P.-Y.; Kaartvedt, S., Røstad, A.; Jones, B. H. *Aquaculture Environment Interactions*, 2018, *10*, 61–77.
[2] Redgrave, L. S.; Sutton, S. B.; Webber, M. A.; Piddock, L. J. V. *Trends in Microbiology*, 2014, *22*(8), 438–445.
[3] Kümmerer, K.; Al-Ahmad, A.; Mersch-Sundermann, V. *Chemosphere,* 2000, *40*(7), 701–710.
[4] de Ilurdoz, M. S., Sadhwani, J. J., & Reboso, J. V. *Journal of Water Process Engineering*, 2022*, 45*, 102474.
[5] The Review on Microbial Resistance. *Wellcome Trust and the UK Department of Health* 2014.
[6] Plhalová, L., Zivna, D., Bartošková, M., Blahova, J., Ševčíková, M., Škorič, M., Marsalek, P., Stancová, V., & Svobodová, Z. *Neuro Endocrinology Letters,* 2014
[7] Nunes, B., Leal, C., Rodrigues, S., & Antunes, S. C. *Water Science and Technology*, 2017*, 3,* 835–844.
[8] Diniz, V., Rath, G., Rath, S., Rodrigues-Silva, C., Guimarães, J. R., & Cunha, D. G. F. *Toxicology Reports* 2021, *8*, 429–435.
[9] Todorenko, D. A., Sidochenko, N. D., Baizhumanov, A. A., Bratkovskaya, L. B., & Matorin, D. N. *Moscow University Biological Sciences Bulletin*, 2023, *78*(3), 172–179

OC17

Hidden costs of beauty: An *in vitro* study on the ecotoxicological impacts of Parabens and Ultraviolet Filters on the bioindicator species *Mytilus galloprovincialis*

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The growing concern over ultraviolet (UV) radiation-induced skin damage has increased the use of photoprotective personal care products (PCPs) containing UV filters, namely ecamsule (ECA), 2-ethylhexyl 4-methoxycinnamate (EHMC) and octocrylene (OC). Parabens, such as propylparaben (PPb) and methylparaben (MPb) are also commonly added to these PCPs to prevent microorganisms' growth and extend the product's shell life. These contaminants enter aquatic environments, posing ecotoxicological risks to marine organisms. We conducted *in vitro* toxicity assessments using S9 subcellular fractions from *Mytilus galloprovincialis* digestive glands (DG) and gills (G) exposed to 0-5000 ng/L of these cosmetic chemicals for 30 minutes. EHMC and parabens decreased antioxidant enzyme activities, while OC increased glutathione peroxidase activity. Carboxylesterases activity was inhibited in G exposed to EHMC and parabens. ECA increased carboxylesterases activity in DG at higher concentrations. Glutathione-S-transferases activity increased in G exposed to MPb and the highest concentration PPb. DG showed sensitivity to EHMC and ECA regarding neurotoxicity and G exhibited neurotoxic responses to EHMC and parabens. EHMC and parabens demonstrated the strongest toxic effects across antioxidant systems, biotransformation pathways, and neurological endpoints. This *in vitro* approach provides a resource-efficient method for preliminary ecotoxicity screening of emerging contaminants.

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OC18

Microplastics as Vector for Pharmaceuticals: Analytical Challenges and Ecotoxicological Risks in Aquatic Systems

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The co-occurrence of microplastics and pharmaceutical residues in aquatic environments raises increasing concerns about their interactions, environmental fate, and potential (combined) ecotoxicological impacts. Due to their high area-to-volume ratio and hydrophobicity, microplastics can sorb and transport pharmaceuticals. Microplastics may, therefore, affect pharmaceuticals' distribution and bioavailability, depending on the chemical interaction, their physicochemical properties, and environmental drivers. If ingested, desorption of pharmaceuticals from microplastics to biological tissues/organs might occur, influencing bioaccumulation and toxic responses across trophic levels [1].

While laboratory studies have provided valuable insights into the mechanisms of pharmaceutical sorption to microplastics—highlighting influences of polymer type, surface area, and biofouling— and on the potential bioaccumulation and ecotoxicological effects on different taxa, critical knowledge gaps persist in understanding these processes under environmentally relevant conditions [2]. Analytical challenges in sampling, extraction, and quantification compromise the assessment of pharmaceutical-microplastics interactions and their (eco)toxicity in natural settings.

This presentation focuses on recent advances addressing the dual role of microplastics as carriers and modulators of pharmaceutical (eco)toxicity. It synthesises evidence of effects on aquatic organisms exposed to microplastic-pharmaceutical mixtures and presents scenarios illustrating varied ecological risks. Key knowledge gaps are identified, emphasising the urgent need for standardised methodologies, advanced analytical tools, and field-based monitoring to characterise real-world exposures accurately. Understanding the interplay between microplastics and pharmaceuticals is pivotal for informing risk assessments, guiding mitigation strategies, and supporting policy decisions to protect aquatic ecosystems from the combined threats posed by plastic and pharmaceutical pollution.

Acknowledgements: CESAM [LA/P/0094/2020] and FCT [CEECIND/01366/2018/CP1559/CT0009].

[1] Santos L.H.M.L.M., Rodríguez-Mozaz S., Barceló D., Microplastics as vectors of pharmaceuticals in aquatic organisms – An overview of their environmental implications, Case Stud. Chem. Environ. Eng. 3, 2021, 100079.

[2] Silva A.L.P., Barceló D., Rocha-Santos T., Pharmaceuticals and micro(nano)plastics in the environment: Sorption and analytical challenges, Trends Environ. Anal. Chem. 44, 2024, e00243.

OC19

New Approach Methodologies predict pharmaceutical pollution

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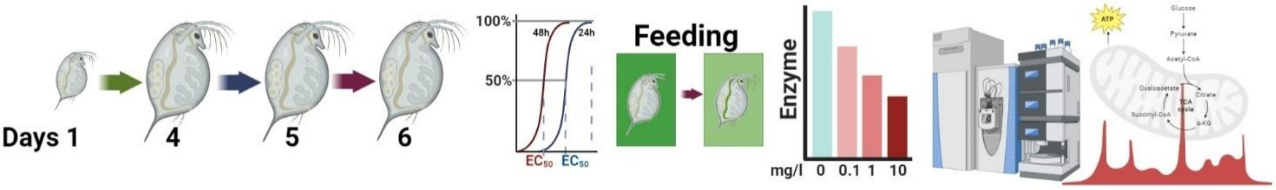
Conventional methods for water monitoring are insufficient to capture the impacts of pollution because of their sensitivity limits, while they also fail to provide mechanistic insight regarding the actions of pollutants. On the other hand, New Approach Methodologies are increasingly introduced as supplementary tools that provide sensitive metrics for pollution assessment. In this context, freshwater sentinel species commonly known as water fleas were used to assess the impact of a pharmaceutical mixture. Daphnids were grown for four days and exposed to a pharmaceutical cocktail which comprised of representatives of commonly encountered pharmaceuticals, and specifically diclofenac, metformin, gabapentin, amoxicillin, trimethoprim, and erythromycin. Combining toxicity curves, phenotypic and molecular endpoints, results showed differences in mortality, feeding, key enzyme activities and metabolic perturbations, thus supporting a distinct pattern in physiological responses of daphnids that could be used to monitor and predict pollution early.



OC21

Reuse of reclaimed water (EU 2020/741) and release of treated effluent (EU 2024/3019) - The selection of priority CECs for monitoring plans.

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Conventional wastewater treatment plants (WWTPs) require additional end-of-pipe treatment steps to ensure that the quality of secondary effluent meets the minimum requirements for water reuse in accordance with local, regional or national laws as well as the recent European Regulation 2020/741 [1]. There is also a need to reduce the levels of contaminants of emerging concern (CECs) (most of them unregulated), as their presence in the aquatic environment is a growing environmental concern [2].

The recent EU directive 2024/3019 [3] requires a quaternary treatment for the large WWTPs and the medium ones placed in areas at risk in order to achieve 80 % of removal for a set of compounds among a listed group or in their absence for site-specific compounds which must be identified. The selection of the relevant CECs to be included in monitoring plans in the area of interest becomes necessary both for the reuse and the release [4].

In this context, the current study aims to prioritize CECs found in the secondary effluent of Italian municipal WWTPs. CECs are ranked on the basis of five criteria: occurrence O, load L, persistence P, bioaccumulation B, and toxicity T, respectively expressed in terms of concentrations in secondary effluent (ng/L), load associated to the secondary effluent and referred to 1000 inhabitants (mg/day/1000 inh), removal achieved in conventional activated sludge systems, octanol-water partition coefficient (Log K_{ow}) and predicted-no-effect concentration in water (ng/L). Due to the very different variability ranges of each of the five criteria, a normalization step is performed by means of a score (1-5) assignment to each of them. The sum of the five scores leads to a final score S for each CEC. The higher the (final) score, the higher the risk associated to the compound. The CECs are then ranked in descending order and those with S greater than 75° percentile are candidate to be considered priority compounds for the area under study.

Based on literature data, 173 CECs belonging to 32 different classes were found in the secondary effluent of Italian WWTPs, of which 34 (approximately 20%) resulted of priority. They include: 17α-ethinylestradiol, 17β-estradiol, fluoxetine, mevastatin, glibenclamide, PFOA and PFOS, galaxolide, and diclofenac (also listed in [3]).

The results of this study refer to a dataset built with literature data for the concentrations, load and removal efficiencies. If experimental investigations are possible for a specific WWTP, the selection may refer to the collected measures of concentrations and resulting loads and removals. In this case, the selection of CECs may better grasp the local peculiarities.

[1] EU Regulation 2020/741 (2020) Regulation (EU) 2020/741 of the European Parliament and of the Council of 25 May 2020 on minimum requirements for water reuse. Off. J. Eur. Union. https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32020R0741&from=EN

[2] Verlicchi, P., Al Aukidy, M., Zambello, E. Occurrence of Pharmaceutical Compounds in Urban Wastewater: Removal, Mass Load and Environmental Risk After a Secondary Treatment-A Review. *Science of the Total Environment* 2012, *429*, 123-155.

[3] EU Directive 2024/3019. Directive (EU) 2024/3019 of the European Parliament and of the Council of 27 November 2024 concerning urban wastewater treatment, Official Journal of the European Union, 2024, https://eur-lex.europa.eu/legal-content/EN/ALL/?uri=OJ%3AL_202403019

[4] Verlicchi, P., Grillini, V., Lacasa, E., Archer, E., Krzeminski, P., Gomes, A. I., Vilar, V. J. P., Rodrigo, M. A., Gäbler, J., Schäfer, L. Selection of indicator contaminants of emerging concern when reusing reclaimed water for irrigation — A proposed methodology. *Science of the total environment* 2023, *873*, 162359

OC22

Advanced Environmental Control Technologies: Integrated Analytical Solutions for Emerging Contaminants

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This presentation provides an overview of the latest analytical technologies developed to detect, characterize, and quantify both known and emerging environmental contaminants. These innovations are crucial for supporting regulators, researchers, and industries in efforts to protect the environment, ensure regulatory compliance, and implement effective remediation strategies.

One of the main areas we will address is the role of heavy metals and metalloid pollutants in environmental degradation and their impact on human health. Through the use of Inductively Coupled Plasma Mass Spectrometry (ICP-MS), we offer valuable insights into the quantification, isotopic fingerprinting, and source tracking of trace metals in environmental matrices such as soil, sediment, and groundwater. This powerful technique is essential for evaluating and optimizing remediation strategies, conducting thorough risk assessments, and ensuring adherence to regulatory standards.

We will also highlight the growing environmental challenge posed by microplastics. Using Micro-FTIR (Fourier Transform Infrared) imaging technology, we present an automated and intuitive workflow designed for the identification, classification, and quantification of microplastic particles, ranging from 10 µm down to 1 µm. This approach offers critical insights into the distribution and impact of microplastics on both aquatic and terrestrial ecosystems, contributing to efforts aimed at understanding and mitigating their environmental footprint.

A particular focus will be placed on PFAS (Per- and Polyfluoroalkyl Substances), widely referred to as "forever chemicals." By employing triple quadrupole LC-MS/MS, we introduce a robust and validated workflow for the targeted analysis of regulated PFAS compounds across complex environmental matrices. Alongside these established pollutants, we recognize the growing concern surrounding new and emerging chemicals. To address this, we turn to Orbitrap-based high-resolution mass spectrometry, which allows for non-targeted screening and suspect analysis, uncovering previously undetected contaminants. The exceptional mass accuracy, resolution, and dynamic range of the Orbitrap platform facilitate the detection of transformation products, novel industrial chemicals, and other emerging environmental threats.

Lastly, we will discuss the continued environmental and health risks associated with Persistent Organic Pollutants (POPs), including polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), and dioxins. Using advanced GC- and LC-Orbitrap methods, we explore both targeted and non-targeted detection strategies to monitor these compounds, enabling both retrospective analysis and real-time surveillance of contamination hotspots.

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OC23

Boosting the reduction of the environmental impact of pharmaceutical products throughout their entire life cycle

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The impact of the pharmaceutical industry on the environment has become a critical issue in recent years due to increases in pharmaceutical consumption and production driven by a general aging population and the rising of healthcare spending.

ETERNAL is an EU funded project that brings together academic, public and private entities to develop and promote more sustainable pharmaceutical practices. With the help of innovative digital tools and using a 'full life cycle' approach, in which each phase of a drug’s life is broken down to identify case studies and potential improvements, ETERNAL aims to address the two principal pollution modalities of the pharmaceutical industry: direct chemical contamination and manufacturing emissions.

Pharmaceuticals (by)-product can directly contaminate the environment through leakages, excretion, improper handling and/or disposal. To mitigate the associated risks, the ETERNAL project will investigate less environmentally harmful products, ecotoxicity and innovative wastewater treatments. Green manufacturing methods such as mechanochemistry, biotechnology, solvent and energy savings will also be explored to reduce emissions and waste.

Overall, by promoting safe and sustainable pharmaceutical practices ETERNAL aim to generate behavioral change, participation and social innovation for a sustainable pharmaceutical industry.

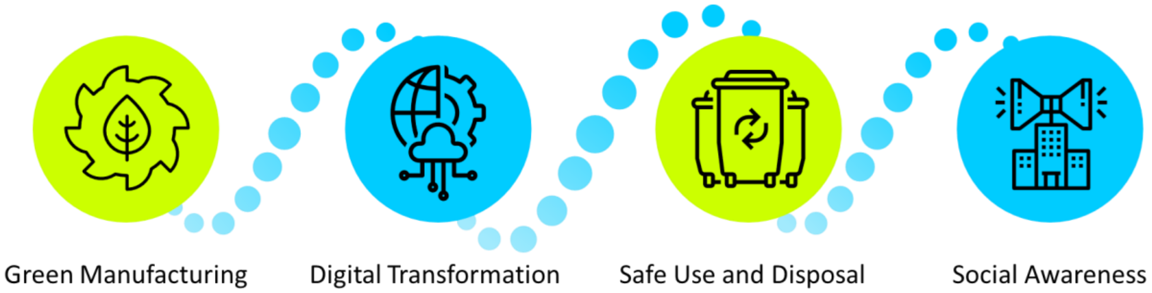

Figure 1: key goals of the ETERNAL project

Acknowledgements: this project has received funding from the European Union’s Framework Program (HORIZON) under grant agreement 101057668.

OC24

The Need for an Early-Stage Sustainability Assessment Methodology

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Life Cycle Assessment (LCA) is a well developed and effective methodology for assessing the environmental impact of projects for chemical and biochemical manufacturing processes including pharmaceuticals. Unfortunately, the level of project detail, necessary expertise of the practitioner, time and cost of an LCA preclude its application very early in a project's life cycle when the greatest benefits in terms of more sustainable route selection can be realised. A simple, comprehensive assessment methodology, specifically designed for the early stages of a project, characterised by incomplete and uncertain information will be introduced. The methodology is designed to aid rational choices between different process development options (see figure 1). The methodology is comprehensive in covering process safety, environmental, economic and social sustainability impacts, energy efficiency, and mass intensity. It also covers the key aspect of technical and scale-up risks, checking if the proposed process can actually work. In the final step a Multi-Criteria Decision Analysis (MCDA) tool [1] is employed taking into account uncertainty by comparing the alternatives as overlapping probability distributions. in the project's team knowledge at the earliest stages of the project.

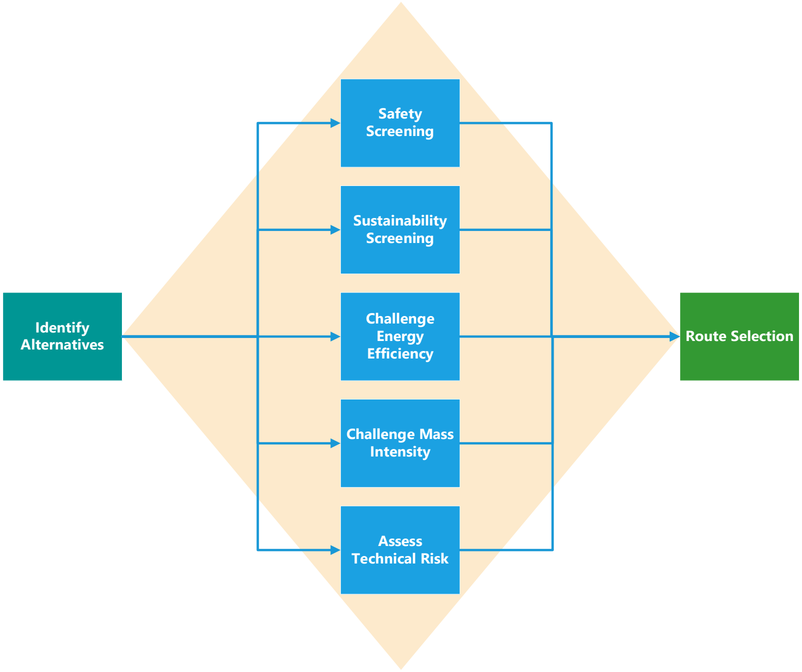

Figure 1: Overview of Methodology for Early-Stage Sustainability Assessment for Chemical and Biochemical Manufacturing Processes

Acknowledgements: This project has received funding from the European Union's Horizon Europe Framework Programme (HORIZON) under grant agreement No 101057668. The work of UK-based Associated Partners has been funded by UK Research and Innovation (UKRI) under the UK government's Horizon Europe funding guarantee.

[1] Henderson, John.; Peeling, Robert. *Open Research Europe* 2024, *https://open-research-europe.ec.europa.eu/articles/4-162/v1*

OC25

Modelling the Emissions of Pharmaceuticals to the Environment

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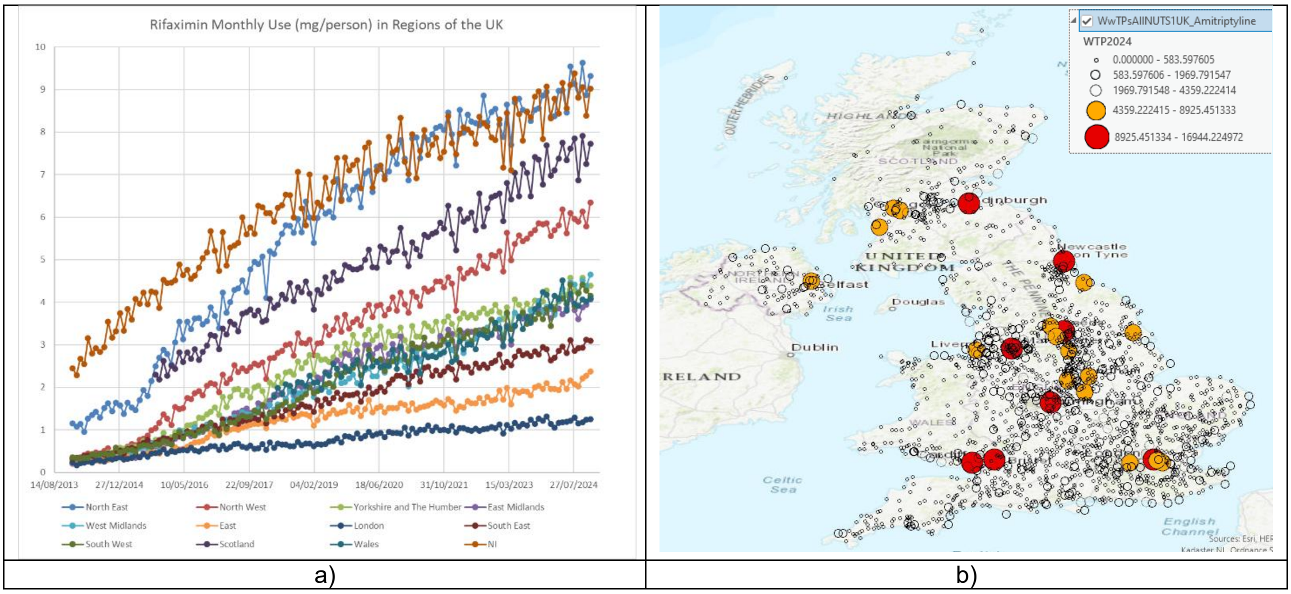
Pharmaceutical consumption is increasing across Europe and globally, raising concerns about releases into the environment and potential impacts on wildlife and human health [1][2]. Yet, environmental monitoring remains limited, and more comprehensive information is needed to assess their environmental concentrations and associated risks. As part of the Horizon Europe project ETERNAL, this study focuses on modelling pharmaceutical emissions, a critical component of broader exposure assessments.

In this study, we developed an emissions model based on general practitioners' prescription data from the UK National Health Service (NHS), targeting selected priority active pharmaceutical ingredients (APIs). Time series of per capita usage were first derived for regions of the country and emissions to wastewater treatment plants (WwTPs) were calculated, accounting for the population served, the fraction excreted unchanged for oral drugs, and wash-off rates for topical formulations. API removal rates within WwTPs were then applied to partition emissions between effluents and sludge.

These transfer rates were mostly derived from literature and the estimated emissions are verified against measured API concentrations in WwTP influents and effluents. Preliminary results (e.g. Figure 1) indicate that the model reasonably estimates emissions, providing reliable inputs for exposure models. The methodology is designed to be scalable and adaptable for application in other European countries.



a) b)

Figure 1: a) Time series of monthly use per capita of Rifaximin for different regions in the UK; b) WwTPs emissions (g) of Amitriptyline [3] in 2024.

Acknowledgements: This work received funding from UK Research and Innovation under the UK government's EUI Horizon Europe funding guarantee for grant agreement No 101057668.

[1] Cleuvers, Michael. (2003). Aquatic Ecotoxicity of Pharmaceuticals Including the Assessment of Combination Effects. Toxicology letters. 142. 185-94. 10.1016/S0378-4274(03)00068-7.

[2] Ternes, T.A., Bonerz, M., Schmidt, T., 2001. Determination of neutral pharmaceuticals in wastewater and rivers by liquid chromatography /electrospray tandem mass spectrometry. J. Chromatogr. A 938, 175 /185.

[3] Rutkowska, A., & Piekoszewski, W. (1999). Chronopharmacokinetics of amitriptyline in rats. Biopharmaceutics & Drug Disposition, 20(3), 117–121

OC26

Hazard Assessment of Pharmaceuticals and their Production Processes: Diclofenac as a case study

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The increasing global demand, consumption and improper disposal and manufacturing of human and veterinary pharmaceuticals have led to an increase in their release in the environment, both in the form of active pharmaceutical ingredients (APIs) and their eventual metabolites. Consequently, a substantial body of scientific literature documents the widespread occurrence and persistent fate of APIs in aquatic and terrestrial ecosystems. To address these challenges, the European Commission (EC) established its Pharmaceutical Strategy for Europe in 2020, while the EC's acceptance of a draft Regulation and Directive in April 2023 to address the environmental impact of medicinal products was paramount. New methodologies, such as compound encapsulation for a controlled release at the site of action and/or bioremediation/enzymatic treatment techniques, are being developed to reduce their environmental impact across their life cycle.

As part of the ETERNAL EU HORIZON project, which is dedicated to advancing the sustainable manufacture, use and disposal of pharmaceuticals, our work directly addresses these issues. In this study, we aimed to evaluate the effects of a novel liposomal encapsulation of diclofenac, before and after enzymatic treatment, as well as the impact of production residues, namely diafiltration waste, using a battery of ecotoxicological assays, while also testing a commercial diclofenac solution for comparison. Enzymatic treatment of the samples was performed using a laccase mediator system comprised of *Trametes hirsuta* laccase (ThL) and the mediator 1-hydroxybenzotriazole (HBT). In addition, the liposomal component was also treated with *Humicola insolens* cutinase (HiC). To this end, an acute toxicity test with *Aliivibrio fischeri* (Microtox), a Yeast Estrogen Screen Assay (YES) and an acute immobilisation test with *Daphnia magna* (OECD 202), were conducted with all samples.

Results demonstrated that the final product and the placebo liposomes, before the enzymatic treatment, may have potentially induced endocrine disruption, as they were able to bind to the estrogen receptor in the yeast. Liposomes loaded with diclofenac produced the highest effect on the bioluminescence by *A. fischeri* and the lowest survival rates in *D. magna*. On the other hand, the commercial diclofenac solution induced the lowest effects in both organisms. The enzymatic treatment of the liposomal encapsulation of diclofenac is expected to reduce toxicity observed in the untreated samples. Even though encapsulation of APIs may solve a current problem, in this case, liposomal encapsulation of diclofenac showed higher toxicity than the commercial formulation, suggesting that the process may affect the targeted and non-targeted delivery of the compound.

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[1] OECD, Test No. 202: Daphnia sp. Acute Immobilisation Test, OECD Guidelines for the Testing of Chemicals, Section 2, OECD Publishing, Paris, 2004, https://doi.org/10.1787/9789264069947-en

Poster
Communications

P1

Optimization and application of an Enzyme Linked ImmunoSorbent Assay for caffeine quantification in water as a marker of anthropogenic pollution

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Anthropogenic pollution is closely associated with human activities and their corresponding domestic and industrial discharges to environment, significantly impacting aquatic ecosystems and, consequently, human health [1]. Caffeine has been identified as a pseudopersistent environmental contaminant, not only due to its long half-life (~10 days) but also because the amounts consumed and released exceed its natural degradation capacity. This persistence is further reinforced by its physicochemical properties, including high stability under variable environmental conditions such as temperature and ionic composition, high solubility and mobility in water, and low volatility.These characteristics make caffeine an effective chemical marker of human-derived pollution, as its presence in aquatic environments is often correlated with other contaminants, including organic residues and pharmaceuticals, which share similar entry pathways. Although wastewater treatment plants (WWTPs) have undergone technological advances, across the different treatment stages (primary, secondary, and/or tertiary), they still face limitations in completely removing emerging contaminants [2]. Regarding the detection and quantification of caffeine, advanced analytical techniques such as Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) and High-Performance Liquid Chromatography (HPLC) offer high sensitivity but are expensive and time-consuming, limiting their routine application in environmental monitoring. As an alternative, immunoassays such as ELISA (Enzyme-Linked Immunosorbent Assay) provide a faster, cost-effective, and accessible approach, albeit susceptible to matrix effects that may compromise accuracy [3]. With the aim of optimizing and applying an ELISA method for the detection of caffeine in environmental water matrices from the Atlantic Ocean at Praia da Barra, brackish water from the Ria de Aveiro, freshwater from the Vouga River, and effluent from the Ílhavo WWTP, three main steps were carried out: i) optimization of the experimental protocol and calibration curve through the combination of different antibodies and caffeine analog tracers, with their respective dilutions; ii) evaluation of matrix effects related to salinity (using NaCl as a representative salt, at concentrations of 10, 20, and 30 g/L) and dissolved organic matter (using commercial humic acids at concentrations of 1, 10, and 20 mg/L); iii) recovery tests in real marine and wastewater samples spiked with caffeine 0.5, 1, and 2 µg/L, to assess potential interferences in method accuracy. Twelve samples were collected and prepared for analysis, and characterized using a multiparametric probe (e.g., pH, salinity, conductivity, dissolved oxygen) and a TOC-VCPH analyzer (e.g., dissolved organic matter). The optimized ELISA proved to be a rapid and accessible tool for the quantification of caffeine in environmentally complex aqueous matrices. Recovery rates indicated that matrix effects did not significantly compromise method accuracy. However, further studies and complementary tests are required for a more rigorous evaluation of method robustness. From an environmental perspective, the results suggest that no significant domestic or industrial wastewater discharges occur directly at the sampling sites, or, if present, their impact is minimal. Despite the low caffeine concentrations detected (0.06 ± 0.01 µg/L), long-term exposure may still pose risks to ecosystem functioning, ultimately affecting the quality of life of aquatic organisms.

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[1] Aliko, V., Turani, B., Multisanti, C. R., & Faggio, C. (2022). Get Rid of Marine Pollution: Bioremediation an Innovative, Attractive, and Successful Cleaning Strategy. *Sustainability*, *14*(18), 11784.
[2] Rout, P. R., Zhang, T. C., Bhunia, P., & Surampalli, R. Y. (2021). Treatment technologies for emerging contaminants in wastewater treatment plants: A review. *Science of The Total Environment*, *753*, 141990.
[3] Jaria, G., Calisto, V., Otero, M., & Esteves, V. (2020). Monitoring pharmaceuticals in the aquatic environment using enzyme-linked immunosorbent assay (ELISA)—a practical overview. *Analytical and Bioanalytical Chemistry* 412, 3983–4008.

P2

Activated carbon from spent coffee grounds for efficient removal of venlafaxine from ultrapure water and wastewater

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In recent decades, the presence of contaminants of emerging concern (CECs) in the environment has become a significant concern due to their persistence, toxicity, and increasing detection in various environmental compartments, particularly aquatic ecosystems [1]. Among the different classes of CECs, pharmaceuticals are considered a priority, as recognized by their inclusion in international monitoring and policy frameworks, including the 2030 Agenda for Sustainable Development [2].

Antidepressants, in particular, have shown a sharp increase in consumption in recent years, in parallel with the rising incidence of depression and related disorders. Venlafaxine (VFX), a widely prescribed antidepressant, is frequently detected in surface waters and wastewater effluents, raising concerns about its potential adverse effects on aquatic organisms and public health. Due to its high chemical stability and low biodegradability, VFX is not effectively removed by conventional wastewater treatment processes [3], leading to its inclusion in the EU Priority Substances Watch List (Decision 2022/1307/EC) [4].

In this context, adsorption has emerged as a promising and efficient technique for the removal of pharmaceutical contaminants from water. It is a physical process based on the adhesion of molecules from a fluid phase onto the surface of a solid adsorbent, typically involving weak, reversible interactions [5]. Among the different adsorbent materials studied, carbon-based adsorbents have gained particular attention due to their high surface area, porosity, and adsorption efficiency, as well as their potential for low-cost production from waste biomass [6].

This study investigates the use of activated carbon (AC) derived from spent coffee grounds (SCG) as an effective and sustainable adsorbent for removing VFX from aqueous matrices. The ACs were produced from SCG via chemical activation using KOH, NaOH, or K_2CO_3 at a 1:1 activating agent/SCG ratio (*w/w*), followed by conventional pyrolysis at 800 °C for 2 hours under an inert nitrogen atmosphere (N_2). Chemical and physical characterization of the three produced materials, followed by kinetic and equilibrium studies for VFX's removal, were conducted. For that purpose, batch adsorption experiments were performed using both ultrapure water and real wastewater collected from a municipal wastewater treatment plant in Aveiro (Portugal), after secondary treatment.

The results demonstrated that the ACs activated with KOH and K_2CO_3 exhibited superior adsorption performance. Notably, the KOH-activated carbon achieved a VFX removal efficiency of 52.0 ± 0.7% in ultrapure water and of 42 ± 3% in real wastewater (with an AC dose of only 25 mg/L), with adsorption equilibrium reached in only 3 hours in both matrices.

These findings highlight the potential of SCG-derived ACs, particularly those activated with KOH, as promising materials for pharmaceutical removal, also promoting circular economy strategies through the valorization of coffee industry waste.

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[1] Samghouli, N.; Bencheikh, I.; Azoulay, K. *Environ. Monit. and Asses.* 2025, vol.197, p.259.
[2] Castillo-Zacarías, C.; Barocio, M. E.; Hidalgo-Vázquez, E.; Sosa-Hernández, J. E.; Parra-Arroyo, L.; López Pacheco, I. Y.; Barceló, D.; Iqbal, H. N. M.; Parra-Saldívar, R. *Science of The Total Environ*. 2021, vol.757, p.143722.
[3] Cerrato-Alvarez, M.; Rioboó-Legaspi, P.; Costa-Rama, E.; Fernández-Abedul, M. T. *Biosens. Bioelectron.* 2025, vol. 267, p.116851.
[4] https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=OJ:L:2022:197:FULL (last access 29/08/25).
[5] Foo, K.Y.; Hameed, B.H. *Chem. Engin. J.* 2010, vol.156, p.2-10.
[6] Mukherjee, A.; Saha, B.; Niu, C.; Dalai, A. K. *J. Environ. Chem. Engin*. 2022, vol. 10, p.108815.

P3

Evaluation of electrochemical degradation using a platinum anode for venlafaxine removal

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Antidepressants have increasingly been recognized as emerging contaminants on a global scale, primarily due to their widespread presence in aquatic environments and their potential to cause detrimental ecological effects. Among these, venlafaxine (VFX), a serotonin–norepinephrine reuptake inhibitor, has raised particular concern due to its documented toxicity toward aquatic organisms [1].

Electrochemical advanced oxidation processes (EAOPs) have emerged as promising technologies for the degradation of pharmaceutical pollutants [2]. However, most studies on the electrochemical degradation of VFX have focused on boron-doped diamond (BDD) electrodes [3]. While BDD electrodes offer advantages such as low background current and a high oxygen evolution overpotential, they also exhibit notable limitations, including delamination, limited scalability, and reduced operational lifetime [4].

The present study investigates the electrochemical degradation of VFX using a platinum (Pt) anode and provides a comparative analysis of its degradation efficiency relative to photolysis and photocatalysis. Platinum was selected due to its intrinsic chemical stability and the availability of reliable surface cleaning protocols, both of which ensured high reproducibility of the experimental conditions.

Degradation experiments were carried out in a 0.1 M Na_2SO_4 electrolyte at pH 9 under galvanostatic conditions, applying a constant current density of 25 mA/cm^2. Under these conditions, a degradation efficiency of 94% was achieved for a 25 ppm VFX solution after 7 hours of treatment.

The degradation mechanism was attributed to the generation of hydroxyl and sulfate radicals within the electrochemical system. The kinetics of VFX degradation followed a pseudo-first-order model, with an estimated rate constant of 0.0084 min^{-1}. Liquid chromatography–tandem mass spectrometry (LC-MS/MS) analysis identified major degradation intermediates, including two isomers with a nominal m/z of 276 and three isomers with a nominal m/z of 294.

Furthermore, an *in silico* toxicity prediction model was employed to assess the environmental impact of the degradation byproducts. The results confirmed the environmental sustainability and potential applicability of the proposed electrochemical treatment method for VFX removal.

[1] De Souza, L.P.; Sanches-Neto, F.O.; Mitsuyoshi Yuki, G., Jr.; Ramos, B.; Lastre-Acosta, A.M.; Carvalho-Silva, V.H.; Silva Costa, A.C. *Process Saf. Environ. Prot.* 2022, *166*, 478–490.
[2] Moreira, F.C.; Boaventura, R.A.R.; Brillas, E.; Vilar, V.J.P. *Appl. Catal. B Environ.* 2017, *202*, 217–261.
[3] Mordačíková, E.; Vojs, M.; Grabicová, K.; Marton, M.; Michniak, P.; Reháček, V.; Bořik, A.; Grabic, R.; Bruncko, J.; Mackuľak, T.; Vojs Staňová, A. *J. Electroanal. Chem.* 2020, *862*, 114007.
[4] Chaplin, B.; Wylie, I.; Zeng, H.; Carlisle, J.; Farrell, J. *J. Appl. Electrochem.* 2011, *41*, 1329–1340.

P4

Environmental Controls on the Sorption of Pharmaceuticals and Their Metabolites in Soils

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Pharmaceuticals and their transformation products are increasingly detected in environmental compartments such as surface water, groundwater, soil, and sediments. Their continuous input arises from both human and veterinary medicine, with consumption in the European Union estimated at 50–150 g per person per year [1]. While many parent pharmaceuticals are only partly excreted unchanged, metabolites such as O-desmethyltramadol (O-DMTRA) and 10,11-dihydro-10-hydroxycarbamazepine (10-OH-CBZ) may enter soils at comparable or even higher levels [2–4].

The persistence and mobility of these compounds in soils are largely governed by sorption processes at the solid–liquid interface. Sorption is influenced by soil composition (e.g., organic matter, clay content, oxides), compound properties (e.g., ionization, hydrophobicity), and environmental factors such as pH, ionic strength, and temperature. For ionizable pharmaceuticals, pH strongly controls electrostatic interactions between charged functional groups and negatively charged soil surfaces, whereas ionic strength may affect competition between sorbate molecules and cations for sorption sites.

In this study, the sorption behavior of tramadol (TRA), carbamazepine (CBZ), and metabolites O-DMTRA and 10-OH-CBZ was investigated using batch equilibrium experiments (OECD 106) with two reference soils of contrasting physicochemical properties. The effects of pH and ionic strength were systematically examined. TRA and O-DMTRA exhibited strong pH-dependent sorption, with retention decreasing sharply above pH 10 as both molecules shifted from charged to neutral forms. Their sorption also declined with increasing ionic strength (using $CaCl_2$), due to competition between Ca^{2+} ions and positively charged analytes for negatively charged soil surfaces. In contrast, CBZ and 10-OH-CBZ, which remain neutral across the tested pH range, showed weak sorption largely unaffected by pH or ionic strength, suggesting the dominance of van der Waals interactions.

Overall, these findings highlight the critical role of soil solution chemistry in controlling the mobility of pharmaceuticals and their metabolites. Ionizable compounds such as TRA and O-DMTRA exhibit much stronger sorption under low ionic strength conditions but may become highly mobile in ion-rich environments, thereby increasing the risk of groundwater contamination. These insights provide valuable input for environmental risk assessment and groundwater protection.

[1] Maszkowska, J.; Kołodziejska, M.; Białk-Bielińska, A.; Mrozik, W.; Kumirska, J.; Stepnowski, P.; Palavinskas, R.; Krüger, O.; Kalbe, U. *J. Hazard. Mater.* 2013, *260,* 468–474.
[2] Bahlmann, A.; Brack, W.; Schneider, R. J.; Krauss, M. *Water Res.* 2014, *57*, 104–114.
[3] Toński, W.; Dołżonek, J.; Stepnowski , P.; Białk-Bielińska, A. *Chemosphere* 2019, *231*, 269–275.
[4] Ebele, A. J.; Abou-Elwafa Abdallah, M.; Harrad, S. *Environ. Int.* 2017, *94*, 50–62.

P5

MINIATURIZATION OF ECOTOXICOLOGICAL TESTS AND THEIR APPLICATION TO ASSESS THE TOXICITY OF ß-BLOCKERS TOWARDS CYANOBACTERIUM *MICROCYSTIS AERUGINOSA*

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Pollution of waters with pharmaceuticals is an emerging problem, as reported by environmental scientist. These pollutants are particularly dangerous because they have high biological activity and affect organisms even at very low concentrations. Thereby these is an concern about its affect entire aquatic ecosystems, from mammals to microorganisms such as algae and cyanobacteria. The latter belong to phytoplankton, which is the basis of the ecosystem and constitutes the basis of the food chain in the aquatic environment. Furthermore, the increase blooms of toxic cyanobacteria are temporally and spatially problematic for people. It is therefore necessary to immediately determine the impact of pharmaceutical contaminants on this group of organisms. For this purpose, ecotoxicological tests are carried out, which are time-consuming and require large expenditures. In this research, we attempted to miniaturize such tests, while taking into account the guidelines of the OECD 201 standard. Miniaturization of ecotoxicological tests is aimed at reducing the amount of reagents, materials, time and workload. The developed tests enable quick testing the toxicity of chemical substances in many concentrations simultaneously in small volumes. The developed method was used to examine the toxicity of pharmaceuticals from beta-blockers group (atenolol, metoprolol and propranolol) towards the *Microcystis aeruginosa*. The results show that toxicity was connected with lipophilicity of target. The test with potassium dichromate as reference substance show applicability of developed protocol.

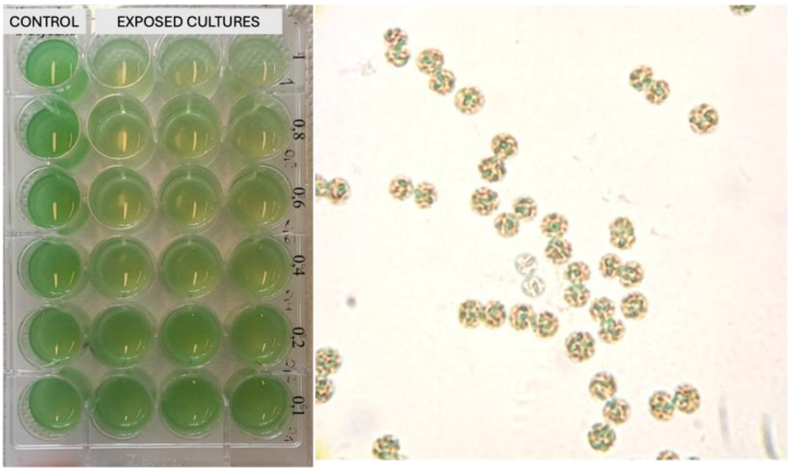

Figure 1: Picture of test plate and microscopic picture of *M. aeruginosa*

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P6

TiO_2 photocatalyst supported on superparamagnetic silica aerogel for sunlight-activated removal of pharmaceuticals from wastewaters

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The pharmaceuticals occurrence in urban streams and rivers of many cities is generally associated to the inefficient treatment of wastewaters regarding these contaminants. This study aimed to synthesize a sunlight-activated titania-silica aerogel photocatalyst with imbedded magnetite nanoparticles for removal of pharmaceuticals in Wastewater Treatment Plants (WWTPs).

First, size-controlled, silica-coated Superparamagnetic Iron Oxide Nanoparticles (SPIONs) were obtained following a previous validated procedure [1]. To obtain the nanoparticles, iron oxide was synthesized by microemulsion, leading to hydrophilic SPIONs, which were after coated with a silica shell (SiO_2), synthesized from TEOS (tetraethyl orthosilicate), to protect against oxidation. The SPIONs would be incorporated into the photocatalyst to facilitate its removal after use, preventing the runoff into waterbodies. Silica gel was prepared by an acid-base catalyzed sol-gel process, from two precursors (80% TEOS and 20% VTMS – vinyltrimethoxysilane), and using ethanol as solvent. Sol-gel route was also used to coat the silica surface with titania (TiO_2), by directly adding TTIP (titanium tetra-isopropoxide) to the sol stage 24 hours after the start of the process. The added volume of TTIP was expected to form TiO_2 after one hour of reaction [2], which would be equivalent to 10% of the aerogel weight. The SPIONs were also added in the sol stage (equivalent to 5% of the aerogel weight), shortly after the base addition, but before the formation of the gel. Finally, after five days of aging, high-temperature supercritical drying with ethanol as supercritical fluid was applied to obtain the desired crystal structures.

Preliminary tests were applied to the photocatalyst in the dark (adsorption test) and under sunlight (photocatalytic test), using ultrapure water and analytical standards of ciprofloxacin (CIP) – antibiotic, and carbamazepine (CBZ) – anticonvulsant, pharmaceuticals usually found in urban streams [3]. The initial concentrations were 10 mg/L for CIP and 20 mg/L for CBZ. The photocatalyst concentration in the water solutions varied from 145 mg/L to 254 mg/L. The adsorption test lasted 2 hours, with *ca.* 4 mL-samples collected at 30-minute intervals. The UV-Vis absorbances showed relevant adsorptions of both pharmaceuticals up to one hour. The photocatalytic test was conducted in Coimbra (Portugal), during an early-summer day, under 28-29 MJ/m^2 (irradiation) and 21-24 °C (air temperature). The photocatalytic test also lasted 2 hours and samples were collected again at 30-minute intervals. However, the UV-Vis absorbances for the photocatalysis of both pharmaceuticals did not show significant improvements in their removal under the applied conditions. HPLC quantification is currently being applied for confirmation. Also, the incorporation of SPIONs has to be optimized for better magnetic removal efficiency. Improvements in the synthesis of this photocatalyst are still necessary, although it is promising for pharmaceuticals removal from wastewater.

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[1] Vaz-Ramos, J.; Cordeiro, R.; Castro, M. M. C. A.; Geraldes, C. F. G. C.; Costa, B. F. O.; Faneca, H.; Durães, L. *Materials Science and Engineering: C* 2020, *115*, 111124.
[2] Romeiro, A.; Azenha, M. E.; Canle, M.; Rodrigues, V. H. N.; da Silva, J. P.; Burrows, H. D. *ChemistrySelect* 2018, *3*, 10915 – 10924.
[3] Rodrigues, F.; Durães, L.; Simões, N. E. C.; Pereira, A. M. P. T.; Silva, L. J. G.; Feio, M. J. *Water Research* 2025, *268 Part B*, 122657.

P7

Occurrence and Risk Assessment of Selected Pharmaceuticals and Their Transformation Products in Northern Poland

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Pharmaceuticals and their transformation products are recognized as emerging contaminants in aquatic environments due to their persistence, biological activity and hence potential ecological effects. The aim of our study was to investigate the occurrence, distribution, and potential risks of selected pharmaceuticals and their transformation products in surface waters and wastewater effluents in Northern Poland. Water samples were collected from rivers, lakes, and wastewater treatment plant outlets and analyzed using LC-MS/MS technique. The concentrations of parent compounds and their transformation products were quantified, and their spatial and temporal variability was assessed. Risk assessment was performed using environmental risk quotients and predicted no-effect concentrations to evaluate potential threats to aquatic organisms based on the performed ecotoxicological studies based on the organisms' representing levels of different biological organization (bacteria, green algae, crustacean and duckweed). The obtained results confirmed the widespread occurrence of several pharmaceuticals and their transformation products, sometimes exceeding parent compound levels, highlighting the importance of including these metabolites in environmental monitoring programs. These findings provide crucial insights into pharmaceutical pollution in Northern Poland and underscore the need for improved wastewater treatment strategies and regulatory measures to mitigate ecological risks.

P8

MXene-Embedded Dummy MIP-Based Electrochemical Detection for the Determination of Nifuroxazide in Environmental Matrices

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Nifuroxazide (NIF) is an orally administered nitrofuran antibiotic used primarily as an antidiarrheal agent [1]. In this study, an MXene-supported electrochemical sensor was developed using dummy molecular imprinting technology and was applied for the determination of NIF in pharmaceutical dosage forms and environmental samples. First, niobium MXene nanoflowers (NbMXene NFs) were synthesized and utilized as nanomaterials. A monomer solution containing nitrofurazone (NIT, 1.0 mM) as the dummy molecule, 3-amino phenylboronic acid (3-APBA, 1.0 mM) as the functional monomer, 2-hydroxyethyl methacrylate (HEMA) as the basic monomer, and ethylene glycol dimethacrylate (EGDMA) as the crosslinker was prepared. After the mixture, to which NbMXeneNFs (1 mg mL^{-1}) was added, was vortexed for 1 min, 20 µL of it was transferred to another tube and 1 µL of initiator was added. 0.25 µL of the prepared solution was dropped onto the glassy carbon electrode (GCE) surface, and photopolymerization was applied under UV light (365 nm, 100W) for 5 min. The developed sensor (NIT/3-APBA/NbMXeneNFs@MIP/GCE) was characterized using scanning electron microscopy (SEM), energy-dispersive X-ray analysis (EDX), electrochemical impedance spectroscopy (EIS), and cyclic voltammetry (CV). In indirect measurements using a 5.0 mM $[Fe(CN)_6]^{3-/4-}$ solution, the linearity range for NIF determination was obtained as 0.075-0.75 pM. The limits of detection (LOD) and quantification (LOQ) were found to be 0.0136 pM and 0.0454 pM, respectively.

The applicability of the NIT/3-APBA/NbMXeneNFs@MIP/GCE sensor was successfully demonstrated for NIF in pharmaceutical formulations and tap water samples. The sensor showed high performance for NIF, even in the presence of 1000-fold interfering agents commonly found in tap water. The high affinity, reproducibility, selectivity, and stability of the developed sensor provide a highly reliable platform for detecting NIF. Additionally, various approaches, Analytical Greenness Metric (AGREE), Analytical Greenness Preparation (AGREEprep), and Analytical Greenness Assessment Tool for Molecularly Imprinted Polymers Synthesis (AGREEMIP), were employed to evaluate the green profile of the developed method.

[1] Koventhan, C., Musuvadhi Babulal, S., Chen, S. M., Lo, A. Y., Senthamil Selvan, C. Mater Today Chem 2024, 35, 101896.

P9

Development of a Nanomaterial-Supported MIP Electrochemical Sensor for Trace Detection of Rimegepant in Environmental Samples

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Rimegepant (RIME) is a calcitonin gene-related peptide (CGRP) receptor antagonist approved by the FDA in 2019, used for the acute treatment of migraine with/without aura, and for the preventive treatment of episodic migraines in adults [1].

In this study, a highly sensitive electrochemical sensor was first designed to detect RIME using the molecularly imprinted polymer (MIP) method. The sensor was developed by electropolymerization (EP) using RIME as the template molecule, 3-thienylboronic acid (3-TBA) as the functional monomer, aniline (ANI) as the comonomer, and a pH 7.4 phosphate buffer solution (PBS) as the supporting electrolyte solution on the surface of a glassy carbon electrode (GCE). Two-dimensional borophene nanoparticles were added to the polymer to enhance the sensor's functionality. Surface and morphological characterizations of the MIP-based electrochemical sensor were performed using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), scanning electron microscopy (SEM), and energy-dispersive X-ray spectrometry (EDX). The highly selective and sensitive determination of Rimegepant (RIME) in standard solutions, commercial serum, and tap water samples using differential pulse voltammetry (DPV) with a redox probe of 5.0 mM $[Fe(CN)_6]^{3-/4-}$ was successfully achieved. After optimization experiments, the calibration range was found to be between 0.25 pM and 2.5 pM, yielding very low limits of detection (LOD) and quantification (LOQ). The recovery studies proved the accuracy of the nanomaterial-supported MIP-based electrochemical sensor. Moreover, the sensor's selectivity was evaluated using common interfering substances.

Additionally, various approaches, including the Blue Applicability Grade Index (BAGI), Analytical Greenness Metric (AGREE), Analytical Greenness Preparation (AGREEprep), and Analytical Greenness Assessment Tool for Molecularly Imprinted Polymers Synthesis (AGREEMIP), were employed to evaluate the green profile of the developed method.

[1] Aggarwal, A.; Akinci, Y.; Gerhardstein, B. L. Braz. J. Otorhinolaryngol. 2025, 91, 4, 101580.

P10

Development of Copper Nanomaterials as Nanozymes for Advanced Water Treatment

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The presence of organic microcontaminants, such as pharmaceutical residues and synthetic dyes, in aquatic environments is a growing global concern. These contaminants exhibit high persistence, resistance to biodegradation, and biological activity toward non-target organisms, even at low concentrations and their continuous input into surface and wastewater systems poses a risk to ecosystems and human health [1]. Conventional wastewater treatment plants are generally ineffective in fully removing these microcontaminants, which has prompted the exploration of advanced treatment technologies to solve this environmental problem [2]. Among them, nanozymes, which are nanomaterials capable of mimicking the catalytic functions of natural enzymes, have emerged as promising strategies, offering advantages such as low cost, high stability under extreme conditions, reusability, and ease of synthesis. Nanozymes with oxidoreductase-like activity are of particular interest, as they can catalyze redox reactions involved in the transformation and degradation of diverse organic molecules, including several pharmaceuticals and dyes [3].

This study focused on the development and characterization of copper-based nanomaterials, and the evaluation of their ability to mimic oxidoreductase activity, to be applied in the degradation of aquatic contaminants. Two types of nanoparticles were successfully synthesized in aqueous media: copper nanoparticles stabilized with glutathione (CuNPs-GSH) and copper selenide nanoparticles stabilized with mercaptosuccinic acid ($Cu_{2-x}Se$-MSA). The synthesis conditions included controlled temperature and pH, followed by purification via membrane filtration or freezing-centrifugation techniques. UV-Vis spectroscopy confirmed the success of the synthesis and scanning transmission electron microscopy (STEM) revealed that CuNPs-GSH consist of mostly spherical particles with an average diameter of 31 ± 4 nm, whereas $Cu_{2-x}Se$-MS are more elongated particles with irregularities on their surface, with average widths of 102 ± 14 nm and lengths of 346 ± 59 nm.

The catalytic activity assays with azo dyes, Methyl Orange and Congo Red, in the presence of sodium borohydride as reducing agent, revealed that both nanoparticles exhibit reductase-like mimetic activity. CuNPs-GSH showed selective activity toward methyl orange while $Cu_{2-x}Se$-MSA preferentially catalyzed the reduction of Congo red. Given the promising catalytic performance and substrate selectivity observed, these copper-based nanomaterials show strong potential as nanozymes for environmental remediation. Future work will focus on evaluating their ability to degrade pharmaceutical contaminants in aqueous matrices, further exploring their applicability in advanced water treatment systems.

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[1] P. Rajak, “Green nanomaterial-based sustainable analysis of contaminant-remediation in wastewater: A bird’s-eye view on recent advances and limitations,” *Sustainable Chemistry for the Environment*, p. 100238, Mar. 2025, doi: 10.1016/J.SCENV.2025.100238.
[2] M. Z. Hashmi, A. Habib, and A. Hasnain, “Removal of antibiotics from wastewater using nanoparticles-based technology: a review,” *Journal of Umm Al-Qura University for Applied Sciences*, pp. 1–9, Aug. 2024, doi: 10.1007/S43994-024-00183-5/FIGURES/3.
[3] W. Wu, C. Peng, Y. Wang, J. Li, and E. Wang, “Building hydrophobic substrate pocket to boost activity of laccase-like nanozyme through acetonitrile-mediated strategy,” *J Colloid Interface Sci*, vol. 680, pp. 785–794, Feb. 2025, doi: 10.1016/J.JCIS.2024.11.021.

P11

Activated Carbon from Brewery Waste: Application in Antibiotic Adsorption and Ecotoxicological Assessment

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The development of affordable and environmentally friendly methods for treating wastewater is crucial to reduce the release of contaminants into aquatic environments, ensuring treatment effectiveness and safety. One promising solution involves the use of carbon-based adsorbents, particularly activated carbon (AC), valued for its large surface area, cost-effectiveness, and versatility across various applications. However, the increasing deployment and functional enhancement of such materials raise questions about their possible environmental release - either as particles or through leachates - and their subsequent effects on aquatic organisms, an issue that remains little explored. In this context, this work aimed to assess i) the adsorptive performance in antibiotic removal from water and ii) the environmental safety of an AC obtained from spent brewery grains (SBG) - a lignocellulosic waste - through microwave pyrolysis with potassium carbonate activation (800 °C, 20 min residence time). The resulting AC (SBG-AC) was sieved (≤ 180 µm) and tested for batch adsorption (kinetic and equilibrium experiments) with three antibiotics frequently detected in the aquatic environments as sulfamethoxazole (SMX), trimethoprim (TMP) and ciprofloxacin (CIP). The tests were conducted, individually and in ultrapure water, at an adsorbent final dosage of 25 mg/L and initial drug concentration of 20 µM. After a contact period of 24 h, the solutions were filtered through 0.22 µm PVDF filters (Whatman) and analysed for the remaining concentration of antibiotic in the aqueous phase by Micellar Electrokinetic Chromatography, using UV-Vis detection at 200 nm. To complement the adsorption assessment, the potential ecotoxicological effects of SBG-AC were investigated using the marine mussel *Mytilus galloprovincialis*, exposed to SBG-AC at a dose of 5, 25 (matching the adsorption dose), and 50 mg/L for 28 days (with weekly water renewal). At the end of the exposure period, biomarkers related to metabolism and oxidative stress were analyzed. The results showed that SBG-AC led to adsorption percentages of 82 ± 4 % for SMX, 84 ± 2 % for TMP, and 94 ± 1 % for CIP. Concerning the toxicological test, the SBG-AC triggered increased metabolic activity in mussels, evidenced by a reduction in energy reserves (glycogen), possibly due to disrupted feeding mechanisms. Also, an increase in the overall antioxidant capability of the organisms was observed. However, at the highest dose tested (50 mg/L), the antioxidant defenses were surpassed, leading to significant oxidative damage, including increased lipid peroxidation and protein carbonylation. These findings emphasize the dual nature of SBG-AC: while it offers a sustainable treatment for wastewater, aligned with circular economy principles, its toxicological impact, especially at higher doses, cannot be ignored. Nonetheless, with proper handling and containment, the risk of environmental contamination can be minimized, allowing the benefits of this circular economy strategy to be realized responsibly.

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P12

Laccase-functionalized biochar from brewery waste for diclofenac removal in continuous stirred tank adsorption systems

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The persistent presence of pharmaceuticals in aquatic environments, namely the anti-inflammatory diclofenac (DCF), represents an increasing risk to human health and aquatic ecosystems. Conventional treatment applied at wastewater treatment plants (WWTP) fail to effectively remove such contaminant, resulting in their continuous release into aquatic systems. Consequently, DCF has been frequently detected in wastewater [1]. In response to this concern, the recent Directive (EU) 2024/3019 [2] mandates the implementation of quaternary treatments in certain WWTPs, by 2045, aiming to remove microcontaminants such as DCF. In this context, adsorption emerges as cost-effective technology, especially when considering the use of sustainable materials like biochar (BC) derived from residual biomass, such as spent brewery grains (SBG). However, BC can exhibit limitations once saturation is reached. To overcome this limitation, modification of BC with laccase (LAC)[3], offers improved stability, reusability, and suitability for continuous processes. LAC is an oxidative enzyme that catalyses the oxidation of a wide range of organic compounds, using molecular oxygen, making it effective in removing of micropollutants from aqueous systems.

This work aims to produce BC from SBG using microwave-assisted pyrolysis, characterize the resulting material, and evaluate its performance for DCF removal under continuous flow condition, in a continuously stirred tank. Additionally, the potential of LAC immobilization on BC (BC-LAC) was explored to enhance DCF degradation. The adsorptive removal of DCF was investigated in three successive stages, with performance evaluated through breakthrough curves. Initially, the effect of adsorbent dose (0.5, 1.0 and 1.5 g L^{-1}) was assessed, using buffered ultrapure water (pH 7.0). Subsequently, the influence of flow rate (1, 2 and 4 L d^{-1}) was examined, under the same conditions. Finally, the performance of BC and BC-LAC was tested using effluent (i.e., water collected after secondary treatment from an urban WWTP in Aveiro South, Portugal), under optimized operational conditions (0.5 g L^{-1} and 1 L d^{-1}). In the case of BC-LAC, the feeding was constantly bubbled with compressed air. The DCF concentration at the continuous system outlet was monitored by High Performance Liquid Chromatography with UV-vis detection, and experimental data from the breakthrough curves were fitted to continuous adsorption models.

The performance of BC was slightly superior in buffered ultrapure water compared to WWTP effluent, with DCF detected only marginally earlier at the outlet, indicating minimal impact on adsorbent saturation. This difference may be attributed to the presence of other organic and inorganic substances in the effluent, which compete for the same adsorption sites. When LAC was incorporated, a slight initial improvement was observed, explained by favourable hydrodynamic conditions and the presence of oxygen inputs supporting enzymatic activity. These results highlight BC-LAC potential, although its application requires adequate operations conditions and consideration of associated costs. Notably, few studies have explored BC from industrial waste for pharmaceutical removal from water, in continuous systems. Therefore, this work fills this gap and provides valuable insights on the applicability of these materials.

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[1] Silva S, Cardoso VV, Duarte L, Carneiro RN, Almeida CMM, 2021. Characterization of Five Portuguese Wastewater Treatment Plants: Removal Efficiency of Pharmaceutical Active Compounds through Conventional Treatment Processes and Environmental Risk. Appl Sci. https://doi.org/10.3390/app11167388

[2] Directive - EU - 2024/3019 - EN - EUR-Lex. https://eur-lex.europa.eu/eli/dir/2024/3019/oj/eng. Accessed 4 Aug 2025

[3] Arca-Ramos A, Eibes G, Feijoo G, Lema JM, Moreira MT, 2017. Enzymatic reactors for the removal of recalcitrant compounds in wastewater. Biocatal Biotransformation 195–215. https://doi.org/10.1080/10242422.2017.1315411

P13

Application of the QuEChERS Method for Extraction of Pharmaceuticals in Dewatered WWTP Sludge

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Sewage sludge produced in Wastewater Treatment Plants (WWTPs) is commonly used in agriculture as a soil fertilizer due to its high content of organic matter and nutrients, such as phosphorus and nitrogen [1]. This practice not only enhances soil fertility and supports crop production but also aligns with the principles of circular economy [2]. However, sewage sludge often contains trace levels of pharmaceutical contaminants, typically in the ng/g to µg/g range [3], which can be introduced into the environment through land application. This poses risks to ecosystems, soil quality, crops, food safety and human health [3].

This study aims to apply the QuEChERS (Quick, Easy, Cheap, Effective, Rugged and Safe) method [4 - 6] to assess its efficiency in extracting nine pharmaceutical compounds from dewatered sewage sludge collected in a WWTP serving 300,000 p.e. Analytes were quantified using High-Performance Liquid Chromatography (HPLC) with fluorescence (FLD) or photo diode array detection (PDA). Method validation included recovery assays using sludge samples spiked with known concentrations (500 ng/g dry matter, n = 3) of the following pharmaceuticals: acetaminophen, atenolol, carbamazepine, diclofenac, fluoxetine, ibuprofen, ofloxacin, propranolol and venlafaxine. The AOAC QuEChERS extraction method was used followed by a clean-up step employing dispersive solid-phase extraction (d-SPE) [4].

Matrix effects were estimated by comparing the area of the analyte standard prepared in the sample matrix with the area of the analyte standard prepared in the solvent (acetonitrile). Suppression of the analytical signal was observed for several pharmaceuticals, with reductions ranging from 1.8% for atenolol and 30% for propranolol. In contrast, signal enhancement was detected for carbamazepine and acetaminophen, with increases of 4.9% and 10.2%, respectively.

Preliminary results revealed that the blank sample exhibited chromatographic peaks at the retention times of several target compounds, suggesting that the sludge is contaminated with certain pharmaceuticals, notably fluoxetine, atenolol, propranolol and venlafaxine. Ofloxacin was detected at very low concentrations following extraction, which aligns with previous findings [7], as this compound exhibits a higher affinity for the aqueous phase. Diclofenac and ibuprofen were not detected in the blank sample nor in the spiked samples, suggesting potential degradation, adsorption to the solid matrix, or losses during the extraction process.

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[1] Bolesta, W., Głodniok, M., & Styszko, K. *IJERPH* 2022, 19, 10246.
[2] Kominko, H., Gorazda, K., & Wzorek, Z. *JWPE* 2024, *63*, 105522.
[3] Wei, H., Tang, M., & Xu, X. *Sci. Total Environ.* 2023, *892*, 164413.
[4] Peysson, W. & Vuillet, E. *J. Chromatogr A* 2013, *1290*, 46 - 61.
[5] Landová, P., Mravcová, L., Poláková, Š. & Kosubová, P. *Environ Sci Pollut Res* Int 2024, *31*, 63946–63958.
[6] Malvar, J. L., Santos, J. L., Martín, J., Aparicio, I., & Alonso, E. *Microchem. J.* 2020, *157*, 104987.
[7] Valverde, M. G., Martínez Bueno, M. J. et al. *Sci. Total Environ.* 2021, *782*, 146759.

P14

Application of magnetic TiO_2/Carbon Quantum Dots for efficient removal of antibiotics from water

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Over the years, the global consumption of antibiotics has increased as well as their presence in the environment mainly due to the discharge of ineffectively treated wastewaters. Such presence plays a major role in the increase of antimicrobial resistance – a major public health problem of the 21st century. The development of efficient and sustainable treatments to remove antibiotics from contaminated effluents has been the focus of extensive research. Solar-driven advanced oxidation processes, especially photocatalysis, are considered promising for the removal of antibiotics from effluents. However, most of the proposed photocatalytic treatments presented in the literature do not allow for an easy recovery of the photocatalyst from the treated water, requiring the application of an ultrafiltration stage that implies higher costs. In this study, a novel photocatalyst based in TiO_2, Carbon Quantum Dots (CQD) and magnetic nanoparticles was produced using a co-precipitation methodology. The produced magnetic TiO_2/CQD composite was tested for the removal of 3 antibiotics (amoxicillin (AMX), sulfamethoxazole (SMX) and trimethoprim (TMP)) under simulated solar irradiation (SolarBox 1500 (Co.fo.me.gra, Italy)). After preliminary experiments to determine appropriate dosage, the photocatalytic performance of the magnetic TiO_2/CQD photocatalyst was tested under different pH (6.00, 7.00, 8.00 and 9.06), dissolved organic matter concentrations (10, 20 and 40 mg L^{-1}), and different water matrices (buffered ultrapure water at pH 8 (phosphate buffer solution (PBS)) and secondary urban wastewater treatment plant (sWWTP) effluent). In parallel, for comparison purposes, the same experiments were run under the same conditions but without the photocatalyst. A photocatalyst dosage of 500 mg L^{-1} allowed for the removal of 47 ± 4% and 44 ± 7% of AMX and TMP, respectively, in 0.4 h irradiation, and 40 ± 2 % removal of SMX in 0.7 h. The pH tests revealed no significant effect for most conditions, except for: (i) lower pH in AMX photocatalysis resulted in significantly lower efficiency; and (ii) higher pH in SMX photocatalysis resulted in significantly higher efficiency. The presence of dissolved organic matter caused a slower removal of all antibiotics and a decrease in the photocatalyst efficiency. This can be due to the inner filter effect of the dissolved organic matter and scavenging/quenching of reactive species. In PBS, the magnetic TiO_2/CQD photocatalyst provided an increase of the photodegradation kinetic rate by 7, 14 and 154 times, respectively for TMP, SMX and AMX. Meanwhile, in sWWTP effluent, the photodegradation kinetic rate increased by 2 times both for TMP and SMX, while external factors hindered the precise quantification of the kinetic rate enhancement for AMX. Furthermore, the magnetic TiO_2/CQD photocatalyst highly impacted the mineralization of the antibiotics reaching 80% mineralization after 15 h irradiation for AMX and TMP and 30 h irradiation for SMX, compared with only 20% mineralization without the photocatalyst for the same irradiation time. Therefore, it is possible to conclude that the applied magnetic photocatalyst is a promising option for a solar-driven advanced treatment of WWTP, allowing for a sustainable removal of antibiotics. This strategy is aligned with Green Chemistry principles and materials circularity, opening the door for the photocatalyst' magnetic after-use recuperation and subsequent reutilization.

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P15

Adsorption and Biocatalysis Synergy for Water Treatment: a laccase-biochar composite for diclofenac removal from water

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Pharmaceutical compounds represent one of the most significant groups of contaminants of emerging concern in aquatic environments, due to their persistence and documented ecological consequences. These microcontaminants often withstand removal by conventional wastewater treatment processes, leading to their accumulation in water bodies and generating risks for both aquatic ecosystems and human health. Diclofenac (DCF), a widely consumed non-steroidal anti-inflammatory drug, exemplifies this issue because of its environmental recalcitrance, potential for bioaccumulation, and toxicological effects on aquatic species. The urgent need to improve wastewater treatment technologies to mitigate the release of such contaminants has been reinforced by the recent European Directive 2024/3019/EU on urban wastewater management. In response, advanced treatment approaches, such as adsorption and enzymatic degradation, have been investigated for their capacity to remove pharmaceuticals from water matrices. Carbon-based adsorbents, namely biochar (BC), have gained significant attention due to their low production cost, enhanced surface area, possible surface functionalization, and strong adsorption properties. In parallel, enzymatic degradation using oxidoreductases like laccases (Lac) offers an efficient catalytic pathway for the transformation of persistent pharmaceuticals. Functionalizing BC with Lac yields a hybrid material that combines adsorption and catalytic degradation, while simultaneously protecting the enzyme from denaturation and extending its operational lifespan. Thus, this work aimed to develop and evaluate a BC enzyme-modified composite for the synergistic removal of DCF from aqueous systems, integrating BC's adsorption capacity with Lac's biocatalytic activity. For this purpose, BC was produced from spent brewery grains (SBG), a major residue of the brewing industry, through microwave-assisted pyrolysis (800 ºC, N_2 atmosphere). The resulting material (SBG-MW-BC) was subsequently functionalized with Lac from *Trametes versicolor* fungi by physical adsorption. The performance of both free Lac and the composite (SBG-MW-BC-Lac) was systematically assessed for DCF removal (initial concentration: 5 mg L^{-1}) under controlled conditions (pH 5 and 7, 25.0 ± 0.1 ºC, 350 rpm) at varying contact times. Remaining DCF concentration in the aqueous phase was quantified recurring to capillary zone electrophoresis (CZE). In parallel, negative-mode electrospray ionization mass spectrometry (ESI(-)MS) and LC-ESI-MS were employed to identify potential transformation products (TP) generated during enzymatic degradation. Overall, immobilization of Lac onto BC was achieved through a straightforward physical adsorption procedure, with the enzyme retaining catalytic activity within the composite over time. The SBG-MW-BC-Lac composite effectively removed DCF via a synergistic mechanism of adsorption and enzymatic transformation. Moreover, ESI(-)MS and ESI(-)MS^2 analyses detected a TP in the free enzyme system that was absent in the composite-treated sample, supporting the hypothesis that the BC matrix may adsorb the TP formed as well as the parent compound. In general, the findings demonstrate that Lac-functionalized BC constitutes a robust dual-functional material for DCF removal. By merging adsorption performance with enzymatic degradation while improving enzyme stability and operational lifespan, this strategy provides a promising approach for enhancing pharmaceutical removal in wastewater treatment applications.

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P16

Evaluating the Normalization Potential of Anthropogenic Markers in Wastewater: Monitoring Influents of German Treatment Plants by ELISA

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Wastewater-based epidemiology (WBE) has emerged as a vital tool for pandemic preparedness, offering early warning capabilities and supporting public health interventions [1]. In Germany, the widespread use of combined sewer systems introduces significant variability in wastewater composition due to rainwater inflow, particularly via street drainage or by indirect discharges from industry. This variability complicates the quantification of pathogens, but also of compounds of health interest such as antibiotics or illicit drugs. To address this challenge, normalization approaches aim to identify suitable markers whose simultaneous measurement allows for the correction of WBE data, thereby improving the accuracy of epidemiological assessments [2].

While human excretion provides relatively stable inputs at the scale of a larger sewage treatment plant's catchment area, many related indicators are either non-specific or degrade during transport. Consequently, the search for anthropogenic markers with sufficiently stable input remains a key focus for improving load calculations in WBE. Selecting appropriate anthropogenic markers requires evaluating the frequency of their occurrence and the variability of their concentrations in wastewater influent across treatment plants of different sizes and regions.

Certain pharmaceuticals—such as carbamazepine, diclofenac, and clarithromycin—as well as commonly consumed substances like caffeine, exhibit sufficiently high concentrations and good chemical stability in wastewater and are not subject to seasonal fluctuations, unlike, for example, hay fever medications.

Antibody-based techniques, particularly the Enzyme-Linked Immunosorbent Assay (ELISA), offer a cost-effective and accessible alternative to chromatographic and mass-spectrometric methods for monitoring trace substances in water. ELISA protocols for detecting the mentioned substances have been successfully developed, requiring minimal sample preparation and no specialized instrumentation [3–5].

This study presents longitudinal data from ELISA-based determination of anthropogenic markers in wastewater samples collected across Germany and evaluates their normalization potential for WBE.

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[1] Phan, T., et al. *Water Res.* 2023, *243*, 120372
[2] Saravia, C., et al. *Front. Public Health* 2024, *12*,1497100
[3] Bahlmann, A., et al. *Chemosphere* 2012, *89* (11), 1278-1286
[4] Carl, P., et al. *Anal. Chem.* 2019, *91*, 12988-12996
[5] Raysyan, A., et al. *Anal. Bioanal. Chem*. 2021, *413*, 999–1007
[6]https://www.rki.de/EN/Topics/Research-and-data/Surveillance-panel/Wastewater-surveillance/wastewater-surveillance-node.html

P17

Removal of sildenafil and tadalafil from water through carbon adsorbents produced from spent brewery grains

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Erectile dysfunction (ED) drugs, namely sildenafil (SILD) and tadalafil (TAD), have attracted a great deal of attention in recent years due to their widespread legal and illegal use around the world and their increasing use by young people for recreational rather than medical purposes [1]. Due to their high stability, these drugs are difficult to degrade or remove effectively using conventional treatments applied in Wastewater Treatment Plants (WWTP). This persistence results in their discharge in effluents, entering surface waters, and negatively impacting humans and ecosystems. Thus, implementing efficient treatments to remove them before effluent discharge is crucial.

In this context, adsorptive treatments have gained renewed attention in recent years due to their effectiveness in removing these recalcitrant contaminants without harmful by-product formation [2]. Carbon-based materials with large specific surface areas, such as activated carbons (ACs), have been widely used for adsorption due to their high porosity, favorable pore size distribution, and potential for surface functionalization [2]. The adsorption performance and cost of ACs depend on factors such as the activation method, precursor material, and thermal treatment. To align with circular economy principles, agricultural and industrial wastes have been explored as sustainable AC precursors, as a way to valorize these underused sources of carbon. In this study, spent brewery grains (SBG), a lignocellulosic waste comprising about 85% of the brewing industry's total waste, were used as the precursor for AC production [3] along with potassium carbonate (K_2CO_3) as the activating reagent. The impregnated raw material then underwent two types of pyrolysis: conventional and microwave-assisted. This approach aimed to evaluate the impact of different thermal treatments on the adsorptive properties of the resulting materials. Microwave-assisted pyrolysis offers a strategic advantage, overcoming the limitations of conventional methods by providing rapid and uniform heating, which results in shorter production times and lower energy consumption [4].

Batch adsorption tests with materials from both pyrolysis strategies, using sildenafil and tadalafil individually were carried out (initial pharmaceutical concentration 5 ppm, 80 rpm shaking, at room temperature). The concentration of the pharmaceutical in the liquid phase was determined by HPLC-UV.

The activated carbon obtained via microwave-assisted pyrolysis demonstrated superior performance, reaching adsorption equilibrium within just 2 hours and achieving removal efficiencies of 90.3% ± 0.08% for SILD and 94.6% ± 2.14% for TAD with an AC dose of only 50 mg/L.

For practical applications, it is essential to evaluate the performance of AC under realistic conditions. This includes assessing matrix and competitive effects on SILD and TAD removal from WWTP effluents. Therefore, adsorption kinetics, equilibrium isotherms, and maximum adsorption capacities of AC-SBG will be determined using biologically treated urban wastewater.

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[1] Zizzamia, A.R.; Tesoro, C.; Bianco, G.; Bufo, S.A.; Ciriello, R.; Brienza, M.; Scrano, L.; Lelario, F. *Case Studies in Chem. and Environ. Engin.* 2024, vol. 9, p. 100708.
[2] Ahmed, M. J. *J. Environ. Manage.* 2017, vol. 190, pp. 274–282.
[3] Sousa, A. F. C.; Gil, M. V.; Calisto, V. *Environ. Sci. Pollut. Res.* 2020, vol. 27, pp. 36463–36475.
[4] Sousa, É.; Rocha, L.; Jaria, G.; Gil, M. V.; Otero, M.; Esteves, V. I.; Calisto, V. *Sci. Total Environ.* 2021, vol. 752, p. 141662.

P18

Chemical Substances Watch List: A Tool for Monitoring and Prevention.

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This work focuses on the Watch List of chemical substances, an important tool for the monitoring and prevention of water pollution in Europe.

It begins by outlining the European Water Framework Directive (2000/60/EC), which introduced the concept of achieving a "good chemical status" for water bodies. To support this, a list of priority substances with environmental quality standards was established. To address emerging pollutants, the Watch List mechanism was introduced (Directive 2008/105/EC, Article 8b), requiring EU countries to monitor selected substances for at least four years.

Environmental risk is assessed through the comparison of: PEC (Predicted Environmental Concentration) PNEC (Predicted No-Effect Concentration) These values help determine whether a substance poses a risk to aquatic ecosystems.

The first national Watch List monitoring campaign in Italy was carried out in 2016. It involved 25 monitoring stations across Italy, targeting substances such as:

Hormones (e.g., 17β-estradiol, estrone), Pharmaceuticals (e.g., diclofenac), Pesticides (neonicotinoids) and UV filters.

Advanced analytical methods were used, including LC-MS/MS and GC-MS/MS, with specific sample preparation techniques (e.g., solid phase extraction).

A special focus is given to neonicotinoid pesticides (imidacloprid, thiamethoxam, clothianidin), which were banned for outdoor use in 2018 due to their toxicity, and completely banned from 2020.

This work emphasizes the importance of ongoing monitoring and the role of the Watch List in identifying and managing emerging environmental threats.

[1] Directive 2000/60/EC of the European Parliament and of the Council establishing a framework for Community action in the field of water policy (Water Framework Directive – WFD).
[2] Directive 2008/105/EC on environmental quality standards in the field of water policy.
[3] Directive 2013/39/EU amending Directives 2000/60/EC and 2008/105/EC as regards priority substances in the field of water policy.
[4] Directive (EU) 2024/3019 of the European Parliament and of the Council on the treatment of urban wastewater.
[5] Italian Legislative Decree No. 172/2015, implementing Directive 2013/39/EU.
[6] European Commission (2015–2023) – Implementing Decisions on the Watch List (Art. 8b of Directive 2008/105/EC). *https://ec.europa.eu/environment/water/water-dangersub/pri_substances.htm*
[7] EFSA (2018) – *Conclusions on the assessment of the risks posed by the neonicotinoid active substances imidacloprid, clothianidin and thiamethoxam to bees*. *European Food Safety Authority Journal.*
[8] Bonmatin, J.-M., Giorio, C., et al. (2015) – *Environmental fate and exposure; neonicotinoids and fipronil*. *Environmental Science and Pollution Research*, 22(1), 35–67.
[9] Riva, F., Zuccato, E., Castiglioni, S. (2019) – *Monitoring emerging contaminants in the aquatic environment: Contribution of the Italian Watch List implementation*. *Science of the Total Environment*, 676, 68–75.

Feeding as a phenotypic endpoint to identify the impact of pharmaceuticals in environmentally low concentrations

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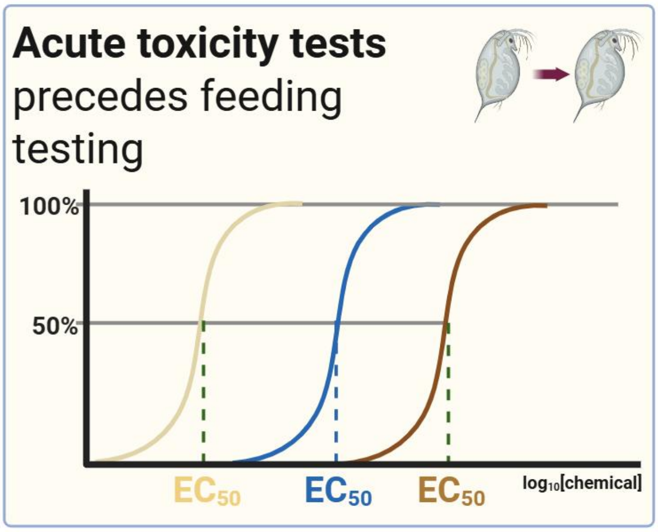
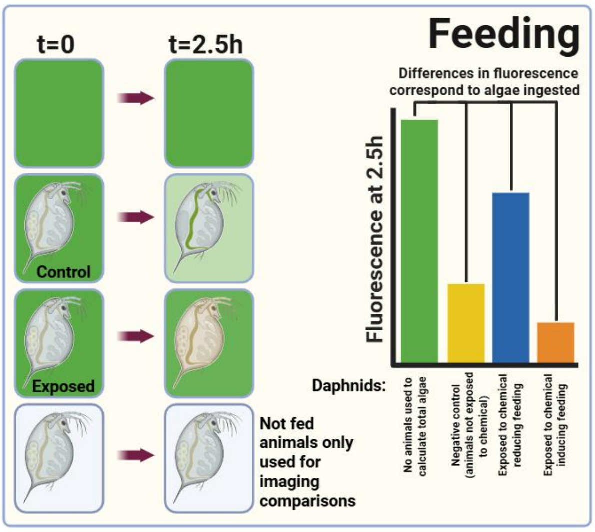
Traditional approaches for monitoring pharmaceutical pollution primarily rely on the chemical analysis and detection of pharmaceuticals in aqueous environments. However, these methods often lack realism and mechanistic insight, prompting a shift toward effect-based methods that provide sensitive endpoints for risk assessment. In this context, daphnids, a freshwater species extensively used in molecular ecotoxicology, offer rapid and non-invasive approaches to assess the impact of pollutants. Among the phenotypic endpoints used, feeding rate is particularly sensitive, as it can indicate physiological alterations even at sublethal concentrations.

Despite its relevance, there has been no standardised method for measuring the feeding rate in daphnids. Existing assays often require large volumes, extensive incubation times, and high animal densities, employing complex techniques such as fluorescence, radiolabelling, or direct counting of ingested cells. These methods can be challenging and labour-intensive, necessitating cumbersome instrumentation. To address these limitations, we developed two robust, fast, and high-throughput assays to assess feeding rate based on the ingestion. Two optimised approaches were tested on neonates of daphnids incorporating an improved feeding protocols using either algae or microplastics as a food source [1-2]. Both protocols were optimised and tested on daphnids following exposure to non-lethal concentrations of a range of pollutants. For feeding, daphnids were incubated with either algae or microplastics, which they ingested as filter feeders. Our findings demonstrated that this new approach could detect significant differences in daphnid physiology even at concentrations below toxicity limits for various pharmaceuticals and pollutants with different modes of action. This confirms that feeding is a very sensitive and non-invasive endpoint for pollution assessment, supporting its integration in Novel Approach Methodologies (NAMs) to support conventional monitoring practices.





[1] Rowan E, Melati Chiappara F, Esmonde H, Grintzalis K. (2025) A miniaturised method for feeding rate in daphnids - A physiology endpoint for risk assessment. NAM Journal, 1:100009

[2] Rowan E, Leung A, Grintzalis K. (2024), A Novel Method for the Assessment of Feeding Rate as a Phenotypic Endpoint for the Impact of Pollutants in Daphnids. Environmental Toxicology and Chemistry, 43: 2211-2221.

P20

The impact of NSAIDs on daphnids – metabolic perturbations as endpoints for the detection of pharmaceuticals in the environment

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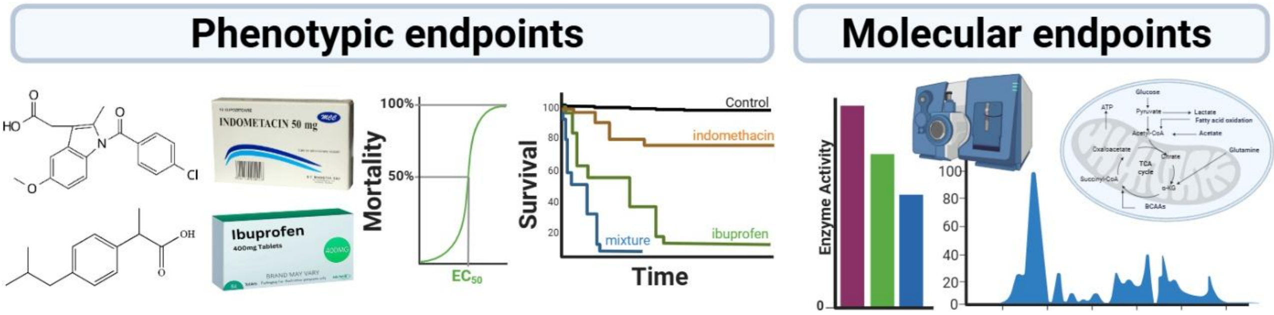
Pharmaceuticals pose a significant threat to the environment with increasing use and access to them. Non-steroidal anti-inflammatory drugs (NSAIDs) are commonly encountered in the aquatic ecosystem in alarming concentrations. In this study, we focused on indomethacin and ibuprofen as two representative NSAIDs. Both NSAIDs were assessed in their pure chemical and commercial forms in single and mixture exposures with toxicity curves, key enzymes and metabolic perturbations as endpoints of the physiology of daphnids. Even at low environmentally relevant concentrations changes in the activities of β-galactosidase and lipase occured. A targeted LC-MS/MS approach revealed distinct metabolic fingerprints as a result of exposure for four generations to the chemical and commercial indomethacin and ibuprofen. Amino acids and biogenic amines were increased following exposure to the chemical mixture of both NSAIDs, commercial NSAIDs and their mixture, while the chemical NSAIDs did have the same impact. This work emphasized the necessity of ecotoxicological studies with transgenerational exposures as an approach to comprehend the effect of pharmaceutical stressors at low exposure concentrations, using molecular responses in physiology. This approach contributes to the broader mechanistic understanding of the ecological implications of these pharmaceuticals in freshwater ecosystems.



P21

Silver selenides as amplifiers for the detection of venlafaxine in water by surface enhanced infrared absorption spectroscopy

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The presence of pharmaceutical contaminants in aquatic environments has become a pressing environmental and public health issue. These compounds, often resistant to degradation, can persist in water bodies, accumulate in living organisms, and interfere with aquatic ecosystems. Their role in promoting antimicrobial resistance is of particular concern, being a growing global threat that directly impacts human health. Addressing this multifaceted problem demands not only effective water treatment strategies, but also sensitive and scalable monitoring techniques capable of detecting trace levels of such microcontaminants.

Conventional analytical methods, while accurate, frequently pose limitations in real-world applications due to their complex instrumentation, high operational costs, and limited adaptability for routine or on-site analysis. As a response to these challenges, surface-enhanced infrared absorption spectroscopy (SEIRA) emerges as a promising alternative. SEIRA enables the detection of analytes at low concentrations by amplifying their vibrational signals, traditionally through the use of plasmonic nanostructures made of gold (Au) or silver (Ag).

Recent studies suggest that silver-based nanomaterials, particularly silver chalcogenides, offer new opportunities as signal enhancers in SEIRA. These materials possess unique surface properties and interaction mechanisms that differ from those of conventional metals, enabling strong local field enhancements. Moreover, they can interact with pharmaceutical molecules through electrostatic forces or surface adsorption, which can localize vibrational modes and result in significant signal amplification.

In this work, the use of silver selenide quantum dots (Ag_2Se QDs) were explored as novel SEIRA amplifiers for the detection venlafaxine as a model analyte. The Ag_2Se QDs were synthesized in aqueous conditions using glutathione (GSH) as a stabilizer and ascorbic acid as a reducing agent. After synthesis, purification steps were applied to minimize spectral interference from unbound stabilizers, enhancing the clarity of analyte–QD interaction assessment. The SEIRA assays were conducted by depositing a mixture of QDs and the analyte to investigate their interaction and assess whether the signal could be effectively amplified. Then, the infrared (IR) spectra were acquired.

Preliminary results indicated that the SEIRA signal could be significantly enhanced, up to 32 times the original signal in specific IR regions, allowing for the detection of venlafaxine at concentrations in the µg/mL range. This work demonstrates the potential of Ag_2Se QDs as signal amplifiers in IR detection through the SEIRA effect. This approach not only expands the range of nanomaterials applicable for vibrational signal enhancement, but also contributes to the development of more sustainable, accessible, and cost-efficient tools for monitoring pharmaceutical contaminants in water.

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P22

UV filters impacts on two sea urchin populations: Atlantic vs. Red sea

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Coastal ecosystems are increasingly vulnerable to the combined impacts of emerging contaminants and climate change. Among these, UV filters, commonly used in personal care products, have raised significant environmental concerns due to their persistence, toxicity, and lipophilic nature. These characteristics promote their accumulation in aquatic environments and, particularly, in resident organisms. Simultaneously, climate change–driven stressors, such as rising temperatures and salinity fluctuations, further threaten the stability of these ecosystems. When these stressors co-occur with the presence of UV filters, their effects may be synergistic or cumulative, amplifying the adverse impacts on marine organisms and undermining the ecological resilience of coastal habitats. This study investigated the cellular effects of octinoxate (EHMC), a widely used UV filter, on two sea urchin species, *Paracentrotus lividus* (Atlantic population) and *Eucidaris* sp. (Red Sea population), under environmentally relevant stress conditions. A 28-day controlled laboratory experiment was conducted, exposing individuals to various EHMC concentrations (50, 500, and 5000 ng/L) under both control conditions (17 and 27 °C; salinity 35 and 40 for the Atlantic and Red Sea populations, respectively) and a simulated climate change scenario (21 °C, salinity 40, applied only to the Atlantic population). Following the exposure period, a suite of biomarkers was analyzed, including metabolic capacity, antioxidant and biotransformation responses, redox balance, cellular damage, and neurotoxicity. Results indicated species- and population-specific responses. *P. lividus*, particularly under the climate change scenario, exhibited marked biochemical alterations, especially under combined exposure to EHMC and elevated temperature, indicating increased susceptibility to warming in conjunction with chemical stress. In contrast, *Eucidaris* sp. displayed more subdued responses to EHMC, suggesting potential physiological tolerance or adaptation to the tested conditions. These findings underscore the ecological risks associated with UV filter pollution, particularly when compounded by abiotic stressors linked to climate change. The interaction between chemical contaminants and environmental variables such as temperature may intensify toxic outcomes, even when individual pollutant levels are moderate. This study highlights the importance of incorporating bioindicator species into integrated environmental risk assessments to capture the complexity of multi-stressor scenarios better.

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P24

Green synthesis of silver and copper QDs as promising radiopharmaceuticals

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Nanomaterials are characterized by their size from 1 to 100 nm, exhibit intriguing properties due to quantum confinement effect, producing unique optical and electronic effects. These properties can be useful for *in vivo* and *in vitro* applications, actively interacting with cellular components at the molecular level [1,2]. Quantum dots (QDs) are crystalline nanostructures from 1.5 to 10 nm, with remarkable electrical and luminescent properties, which give them a wide variety of applications in the biological field, due to the small size [3] including biosensing, drug delivery and bioimaging [4]. However, the toxicity of QDs due to the presence of heavy metals, hazardous components and organic solvents limits their use in the medical field. Traditional synthesis methods provide QDs of the correct size and morphology, but they contain compounds that are hazardous to the environment and human health; they also use expensive techniques and high temperatures. [3,4]. Currently, there is concern about minimizing toxicity and increasing the biocompatibility of QDs, optimizing new synthesis methods without organic solvents or with high toxicity [5].

Silver chalcogenides QDs have been the subject of several studies due to their non-toxic properties and potential use in the biomedical field, with different production methods [6]. On the other hand, copper has been extensively used to produce radiopharmaceuticals, enhancing the cancer treatment outcomes. Cu has short, medium, and long half-life isotopes, making it a suitable element for diagnosis and therapy. As their properties are identical, this element allows the same radiopharmaceutical to be suitable for diagnosis or therapy, simply by changing the appropriate isotope [7].

There is currently a growing interest in the green synthesis of nanoparticles, methods that are less expensive, and that use non-toxic, environmentally friendly solvents, and mild experimental conditions. To reduce the environmental impact of the synthesis of QDs, they can be prepared in water medium, and the traditional reducing agents and precursors could be replaced by biomolecules. Environmental sustainability is the greatest attribute of these techniques, but they require improvements in terms of yield, uniformity, and scale-up [3].

This work has the aim of developing new radiopharmaceuticals based on Ag- and Cu- QDs produced in aqueous medium. Herein, AgCuSe QDs are being prepared adapting the simple aqueous synthesis method of Ag_2Se QDs [5]. Different Ag:Cu molar ratios are being tested to produce QDs with optimized optical properties, The QDs were characterized by the absorption and fluorescence spectra and emitted photoluminescence.

This synthesis method, in addition to not using toxic and expensive solvents, uses only water, is carried out without using expensive technologies at a mild temperature and is fast. Given the low toxicity to humans and the environment, we intend to continue using aqueous synthesis of Ag- and Cu-based QDs for use *in vitro* and *in vivo* studies for cancer imaging and radiotherapy.

[1] Coronado A.G.*et al. International Journal of Molecular Sciences* 2025, *26*, 2633.
[2] Aisha A.; William G. P. and Ghaleb A. *Nanomaterials 2023, 13, 2566.*
[3] Moradialvand, Z.; Parseghian; Rajabi, R. R. *Journal of Hazardous Material Advances* 2025,*18*, 100697.
[4] Rivaux, C. *et al. The Journal of Physical Chemistry C* 2022, *126*, 20524.
[5] Viegas, I.M.A. *et al. New Journal of Chemistry* 2022*, 46,* 21864.
[6] Sharma, A.; Sharma, R.; Thakur, N.; Sharma, P.; Kumari, A. *Physica E: Low-dimensional Systems and Nanostructures* 2023,*151,* 115730.
[7] Kręcisz, P. *et al. Journal of Medicinal Chemistry,* 2025*, 68, 2356*

P25

Synthesis of nadifloxacin derivatives for further ecotoxicological studies

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Fluoroquinolones (FQs), a widely used class of antibiotics, are frequently detected in environmental matrices due to their persistence and incomplete removal during wastewater treatment [1]. Nadifloxacin (NAD) is a chiral FQ prescribed in a racemic form for the topical treatment of mild or moderate inflammatory forms of acne vulgaris. Levonadifloxacin (LNAD), the *S*-enantiomer of NAD, is 250 times more potent than the *R*-isomer [2], Recently, alalevonadifloxacin mesylate, a prodrug of (LNAD), was developed to enhance the oral bioavailability of LNAD, being used to treat infections caused by gram-positive bacteria, including methicillin-resistant *Staphylococcus aureus* [3].

Understanding the stereochemical complexity of NAD and its alalinate diastereoisomeric derivatives, it is crucial for accurate ecotoxicological risk assessment, as the isomers can exhibit distinct bioactivity, degradation pathways, and toxicity profiles [4].

The synthesis of well-defined NAD derivatives enables detailed investigations into these stereoselective behaviours and helps clarifying their environmental fate and biological interactions. Thus, this work aimed to synthesise the alaninate derivatives of both enantiomers of NAD and to explore the influence of the *L* and *D* alanine derivatives of NAD in ecotoxicity. The achievement of how each stereoisomer behaves under ecotoxicological conditions bridges synthetic chemistry with environmental science, ultimately supporting more sustainable pharmaceutical development and pollution mitigation efforts.

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[1] Kümmerer, K. *Chemosphere* 2009, *75* (4), 417-434.
[2] Bhagwat, S. S.; Nandanwar, M.; Kansagara, A.; Patel, A.; Takalkar, S.; Chavan, R.; Periasamy, H.; Yeole, R.; Deshpande, P. K.; Bhavsar, S.; et al. *Drug Design Development and Therapy* 2019, *13*, 4351-4365.
[3] Mehta, Y.; Mishra, K.; Paliwal, Y.; Rangappa, P.; Sinha, S.; Bhapkar, S.*Critical Care Research and Practice* 2022, *2022*, 1-13.
[4] Ribeiro, A. R.; Castro, P. M. L.; Tiritan, M. E. *Environmental Chemistry Letters* 2012, *10* (3), 239-253.

P26

Do Layered Double Hydroxides Reduce Naproxen Effects to Zebrafish *Danio rerio*?

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Inorganic nanoengineered drug delivery systems (NDDS) were initially developed to enable the controlled release of active pharmaceutical ingredients, ensuring optimal therapeutic concentrations within the organism. However, with their increasing use, these systems may ultimately reach wastewater streams. Unfortunately, conventional wastewater treatment plants (WWTPs) do not remove nanomaterials effectively, due to their physicochemical compatibility. As a result, their environmental fate raises concerns about their possible interactions with aquatic organisms and the induction of unintended biological effects.

Given these challenges, it is essential to conduct a comprehensive evaluation of the effects caused by pharmaceuticals in both their free and nanostructured forms. Such studies are crucial to improve the accuracy of environmental risk assessment (ERA), necessitating the development or adaptation of standardised testing protocols and the refinement of risk-based regulatory frameworks.

The present study aims to assess the effects of naproxen sodium, a widely used pharmaceutical, in its soluble form and intercalated into layered double hydroxides (LDHs), using the zebrafish model (*Danio rerio*). Naproxen was intercalated into magnesium–aluminium LDHs (Mg-Al-LDHs), anionic clays broadly employed in controlled-release applications or NDDS. The resulting nanostructured systems were characterised. Their morphology and elemental composition were analysed via transmission and scanning electron microscopy (TEM, SEM-EDX). Structural and chemical properties were evaluated using attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) and X-ray diffraction (XRD). Drug loading and release profiles were quantified using ultraviolet–visible (UV–Vis) spectroscopy.

For ecotoxicological evaluation, *D. rerio* embryos were exposed to aqueous solutions of naproxen sodium salt and dispersions of LDH-intercalated naproxen, following the OECD 236 Fish Embryo Acute Toxicity (FET) test protocol. Endpoints such as NOEC, LOEC, LC_{50} and the occurrence of developmental malformations were determined. Additionally, biochemical markers, such as acetylcholinesterase (AChE), glutathione S-transferase (GST), and catalase (CAT), as well as behavioural responses, were assessed at 120 h post-fertilisation. Finally, genotoxicity was assessed by evaluating DNA damage through the comet assay.

The results confirmed the successful intercalation of naproxen into the LDH layers and revealed distinct ecotoxicological profiles for the soluble and intercalated forms. This ongoing study presents a novel and thoroughly characterised NDDS that is less toxic to zebrafish embryos and does not cause behavioural impairment to the larvae, nor neurotransmission impairment. This work shows that the immobilisation of drugs in NDSS decreases their toxicity and seems to be a sustainable way to decrease the risks to the aquatic environment. It provides valuable data to support the environmental hazard assessment of naproxen sodium and its nanoformulation. Ultimately, these findings will aid in refining ERA approaches and promoting safer pharmaceutical practices with reduced ecological impacts.

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Development and Validation of an Enantioselective SPE-LC-MS/MS Method for Monitoring Fluoroquinolones in the Environment

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Antibiotics have been closely related to the spread of antimicrobial resistance and have been detected in aquatic compartments at concentrations typically ranging from ng/L to µg/L [1]. Several antimicrobials have been included in recent European legislation, namely fluoroquinolone (FQ) antibiotics, represented by ofloxacin (included in the watchlists of Decisions (EU) 2022/1307 and 2025/439 [2,3]), and by ciprofloxacin (suggested to be included in the upcoming amending Directive to Directives 2000/60/CE, 2006/118/EC, and 2008/105/EC [4]). Considering that several of these pollutants are chiral and that their enantiomers can have different bioactivities [5], the monitoring of water samples should distinguish between enantiomers. Indeed, the stereoselectivity of environmental processes may lead to different enantiomers concentrations and enantiomeric fractions, a challenging topic in analytical chemistry that remains poorly explored [5,6].

Solid-phase extraction (SPE) followed by analysis using Liquid Chromatography coupled to tandem Mass Spectrometry (LC-MS/MS) has remained a powerful procedure for monitoring trace contaminants in environmental water samples [1,6]. Thus, the main objective of this work was to obtain a stereoselective SPE-LC-MS/MS method targeting FQs and some metabolites or transformation products.

After testing different chiral stationary phases, a cellulose-based chromatographic column was selected. The optimized chromatographic conditions, which included preliminary trials for mobile phase, flow rate, and temperature selection, allowed the separation of 12 achiral and 16 chiral FQs, with enantioseparation achieved for 6 compounds: flumequine, ofloxacin, N-oxide ofloxacin, desmethyl-ofloxacin, nadifloxacin, and prulifloxacin. Additionally, a SPE procedure using OASIS® HLB cartridges was adapted from literature [1], in order to preconcentrate the targeted FQs from environmental samples prior to analysis. This SPE-LC-MS/MS method is currently under validation for different aqueous matrices and will be applied to the monitoring of FQs in environmental water samples, contributing valuable progress both for environmental monitoring and for defining future strategies addressing this issue.

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[1] Maia, A.S.; Paíga, P.; Delerue-Matos, C.; Castro, P.M.L.; Tiritan, M.E. *Environ Pollut* 2020, *259*, 113927.
[2] Decision 2022/1307 *Official Journal of the European Union*, 2022, *L 197*, 117-121.
[3] Decision 2025/439. *Official Journal of the European Union*, 2025, *L* series.
[4] Proposal for a Directive of the European Parliament and of the Council, COM/2022/540 (2022).
[5] Kasprzyk-Hordern, B. *Chem Soc Rev* 2010, *39*, 4466-4503.
[6] Ribeiro, A.R.; Santos, L.H.M.L.M.; Maia, A.S.; Delerue-Matos, C.; Castro, P.M.L.; Tiritan, M.E. *J Chromatogr A* 2014*, 1363*, 226-235.

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SPE-LC-MS/MS method for the simultaneous determination of chiral and achiral fungicides in drinking water

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Fungicides are organic compounds, many of them chiral, used in diverse applications. Despite their beneficial effects in controlling fungal plagues and treating diseases, their widespread use has led to their detection in the environment, typically at concentrations of up several hundreds of ng/L [1,2]. Consequently, fungicide contamination is an increasing global environmental concern, due to the risks it poses to non-target organisms and human health, as well as its links to antimicrobial resistance [3]. In the case of chiral fungicides, their enantiomers can show different bioactivity, including toxicity and degradation. Thus, monitoring their enantioselective occurrence in the environment is very important to understand their environmental behavior and for conducting accurate risk assessments, a topic still understudied [2-4].
Given that, this work presents an enantioselective analytical method developed for monitoring fungicides in water, using a chiral polysaccharide-based column in reverse elution mode. This method was first optimized by liquid chromatography with diode array detection (LC-DAD) and then adapted to LC coupled with tandem mass spectrometry (MS/MS) to analyze trace concentrations of a group of five chiral azole fungicides (ipconazole, metconazole, penconazole, tebuconazole, and tetraconazole) and one achiral azole fungicide (fluconazole). In addition, solid phase extraction (SPE) experiments were carried out to optimize the best conditions for the recovery of these fungicides. The SPE-LC-MS/MS method was validated then applied to monitor fungicides and their enantiomeric fractions in drinking water samples.

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[1] Wang Y, Wan Y, Li S, He Z, Xu S, Xia W. *Water Res*,2023, 247, 120724
[2] Zhu J, Ouyang W, Guo Z, Liu X, He M, Li Q, Liu H, Lin C. *Environ Int*, 2023, 171, 107697
[3] Draskau MK, Svingen T. *Front Toxicol*, 2022, 4, 883254, 2022
[4] Ribeiro C, Ribeiro AR, Maia AS, Tiritan ME. *Symmetry*, 2017, 9, 215

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Selection of ofloxacin-degrading microorganisms from activated sludge microbiota

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Wastewater treatment plants (WWTPs) are generally unable to efficiently remove pharmaceutical residues, including antibiotics (ABs), from wastewater. This results in the discharge of these residues in the effluents, which is a major pathway for these contaminants to enter aquatic environments [1]. Among ABs, fluoroquinolones (FQs) are especially of concern due to their widespread use, chemical stability, and toxicity. Their recalcitrance in WWTPs is associated with the difficulty of degrading organofluoride compounds through conventional treatments, which contributes to their pseudo-persistence and increases the risk of ecological disruption and potential human health impacts [2,3]. Due to these challenges, FQs have been included in the European Watch Lists, with the most recent Decision 2025/439/EU listing ofloxacin (OFL) for Union-wide monitoring [4]. Furthermore, as a chiral compound, OFL may display enantiomer-dependent bioactivity, which adds complexity to its environmental behavior and its role in the dissemination of antimicrobial resistance [5].

This study aims to identify a bacterium or bacterial consortium, isolated from activated sludge of a pharmaceutical industry WWTP, capable of degrading OFL, and to investigate the enantioselective mechanisms involved in FQs degradation. Different nutrient sources (e.g., yeast extract) and OFL concentrations (64 and 170 mg/L) were tested in inoculated mineral medium to enrich OFL-degrading microorganisms, with 64 mg/L matching the highest EUCAST MIC where resistant isolates persist [6], and 170 mg/L providing 100 ppm of organic carbon from OFL. Microbial growth was monitored by optical density, while OFL degradation was assessed using high-performance liquid chromatography with fluorescence detection, alongside measurements of fluoride release. This work is ongoing, but the results may represent important advances in the identification and isolation of OFL-degrading bacteria, as well as in understanding their behavior towards chiral compounds and the underlying degradation mechanisms.

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[1] Manaia C. M., Macedo G., Fatta-Kassinos D., Nunes O. C. *Appl Microbiol Biotechnol*. 2016. 100, 1543-1557.
[2] Pauletto M., De Liguoro M. *J. Xenobiot*. 2024. 14, 717-752.
[3] Maia A.S., Castro P. M. L., Tiritan M. E. *Journal of Chromatography B*. 2016. 1029–1030, 174–183.
[4] *Commission Implementing Decision 2025/439*. Official Journal of the European Union, L. 2025.
[5] Kasprzyk-Hordern B. *Chem. Soc. Rev*. 2010. 39, 4466–4503
[6] *European Committee on Antimicrobial Susceptibility Testing* (EUCAST). MIC distributions for ofloxacin. 2025. Available from: https://mic.eucast.org/

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Epirubicin-induced DNA damage and gene expression alterations in zebrafish early life stages

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Antineoplastic agents (AA) can end up in the aquatic environment through the hospital and domestic wastewater, partially transformed or even unchanged, via human excretion. It is known that AA can exhibit cytotoxicity at low concentrations, posing potential threats to aquatic organisms. Epirubicin, an anthracycline drug, acts by suppressing DNA and RNA synthesis, and approximately 11% of the unmetabolized form is excreted via urine within 24 h. Detecting antineoplastic agents in the environment presents significant challenges due to their low concentration and potential for transformation into various metabolites and degradation products. Thus, this study aims to assess the physiological and sub-cellular effects of epirubicin in eggs/larvae of *Danio rerio*.

The exposure followed the OECD 236 Fish Embryo toxicity protocol, and mortality, hatching delay, and malformations (e.g., pericardial oedema, incomplete yolk sac absorption, and tail deformities) were recorded during 96 h. DNA damage (evaluated through the comet assay) and gene expression (RT-qPCR) were assessed after 96 h of exposure, while neurotoxicity and oxidative stress-related biomarkers and locomotor behavior were examined at the end of the 120 h exposure period. The quantification for epirubicin in zebrafish media over the test period were assessed by High-Performance Liquid Chromatography with fluorescence detection (HPLC-FLD).

Epirubicin causes 50% of mortality and malformations at a nominal concentration of 64 and 7 mg/L, respectively. DNA damage ranging from 30 to 50 % was observed in zebrafish larvae exposed to concentrations above 61 µg/L, as indicated by tail DNA analysis. No neurotoxic or oxidative stress or alterations in locomotor behavior were detected in *D. rerio* larvae at concentrations up to 206 µg/L. Regarding gene expression, epirubicin exposure (500 µg/L) led to a downregulation of tp53 and catalase gene expression, alongside a significant upregulation of cyp1a, suggesting activation of xenobiotic metabolism pathways.

These findings provide valuable insights into the physiological and sub-cellular effects promoted by AA in aquatic organisms and may assist in their future environmental hazard and risk assessment.

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Selective antibacterial effects of fluoroquinolones on wastewater bacteria

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Conventional wastewater treatment plants (WWTPs) are not designed to effectively remove micropollutants such as pharmaceutically active compounds, including antibiotics [1]. Many of these compounds persist through standard processes due to their high chemical stability, limited biodegradability, and affinity for particulate matter. Sub-inhibitory concentrations of antibiotics in WWTPs may promote the selection of antimicrobial-resistant bacteria and genes, with these facilities acting as reservoirs and hot-spots for horizontal gene transfer, contributing to antimicrobial resistance (AMR) in aquatic systems [2]. Fluoroquinolones (FQs) are of particular concern due to their extensive use in human and veterinary medicine related to their broad-spectrum antimicrobial activity. Moreover, their chiral nature adds complexity, as enantiomers may differ in antimicrobial potency, environmental persistence, and toxicity [3,4]. This study focused on evaluating the selective antibacterial effects of two FQs representatives: ofloxacin (Oflo) and flumequine (Flu). To this end, bacterial biomass was collected from a municipal WWTP, as well as from upstream and downstream sites of the receiving river, filtered, and subsequently exposed to minimum inhibitory concentrations (MICs) levels of Oflo (0.3 mg/L) and Flu (2.5 mg/L), as well as to slightly higher concentrations of 0.5 mg/L and 4.0 mg/L, respectively. Following exposure, bacterial strains were isolated using a selective culture media, Chromogenic Coliform Agar, to differentiate and enumerate coliforms and *Escherichia coli*, with subsequent purification of obtained strains in Plate Count Agar. Pure isolates were then subjected to molecular taxonomic identification via 16S rRNA gene sequencing, allowing for phylogenic characterization and assessment of potential taxon-specific responses to FQs. It was possible to isolate 108 pure bacterial strains, and the results showed that the most frequently isolated bacterial strains belonged to *E. coli* (75%), consistent with its prevalence in wastewater environments. A greater diversity of bacterial isolates was observed upstream of the WWTP due to the natural environment harboring a wider range of microbial niches, whereas the selective pressures within the facility favor only microorganisms adapted to high nutrient loads and chemical stressors. Antimicrobial susceptibility testing was conducted to evaluate the resistance patterns of the isolated bacterial strains when exposed to the selected FQs. This study aids in better understanding the selective effects of FQs on environmental bacteria and their potential role in AMR and serves as a foundation for enantioselective assays. The results obtained provided deeper knowledge on the environmental fate and ecological impact of chiral antibiotics.

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[1] S. -H. Lee et al. (2019). Journal of Water Process Engineering 31, 100828.
[2] M. C. La Rosa et al. (2025). Antibiotics 14(2), 131.
[3] J. K. Stanley et al. (2009). Integrated Environmental Assessment and Management 5(3), 364-373.
[4] S.W. Smith (2009). Toxicological Sciences 110(1), 4-30.

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Incorporation of TiO_2/CQDs into polymeric fibers for the photodegradation of amoxicillin in water

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The growing overuse of antibiotics and the ineffective treatment of urban wastewater are allowing certain drugs, such as antibiotics, to get into rivers, lakes, and other water sources. This not only affects the quality of drinking water but also poses a real threat to the ecosystems, affecting animal and human health. One of the biggest concerns is the rise of antimicrobial resistance, which is becoming a serious global issue.

To develop a new eco-friendly water treatment for the removal of water pollutants such as antibiotics, some research has been focusing on the application of advanced oxidation processes and, especially, the application of sunlight-based treatments to help break down and remove contaminants from water. The application of solar driven photocatalysts has shown high potential to faster this process. Among them, materials like titanium-based nanocomposites and carbon quantum dots (CQD) have shown potential in speeding up this process. However, the challenge lays in the efficient application, recovery and reuse of the photocatalyst.

Therefore, in this study, to create a practical photocatalytic process, titanium oxide (TiO_2) with CQD incorporated (TiO_2/CQD) photocatalyst was combined with polymeric fibers and tested for the removal of amoxicillin (AMX), a specific target antibiotic. After fiber selection, TiO_2/CQD nanocomposites were incorporated into polycaprolactone (PCL) nanofibers, with a ratio of 2:1 fibers:photocatalyst (*w*/*w*). The photocatalysis of AMX (10 mg/L) in phosphate buffer solution (PBS, 0.001 mol/ L, pH = 8) was evaluated using 1.5 g/L of fiber/photocatalyst. The samples were irradiated for 2 hours under solar simulated irradiation. and then analyzed by reverse phase High Performance Liquid Chromatography with UV detection.

The results showed that this approach accelerated the degradation of AMX up to 18 times, decreasing the half-life time from 62 ± 1 h (without catalyst) to 3.45 ± 0.03 h (in the presence of fiber/photocatalyst). These results are an indication that the application of PCL/TiO_2/CQD fibers can be a promising and sustainable approach to remove antibiotics from water environments.

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Removal of antibiotics on chitosan-based adsorbents: a computational study

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The contamination of water with pollutants has significant impact on the health of all organisms that live in the aquatic environment. Water contamination is mainly caused by the release of various substances such as antibiotics. Although antibiotics have been extensively used to treat bacterial infections in both humans and animals, the overuse of antibiotics has resulted in their dissemination throughout the environment, making them one of the most concerning emerging pollutants. Therefore, materials that can perform water remediation are major importance[1]. Among the several methods for the removal of contaminants, adsorption has proven to be the most economical, viable and highly effective. However, commercially available adsorbents have high costs and potential sustainability issues[2]. In contrast, chitosan is a naturally derived polysaccharide obtained from crustacean waste, making it very abundant, non-toxic, unexpensive and biodegradable[3]. The presence of free hydroxyl and amino groups makes the chitosan a good adsorbent. However, the removal of antibiotics by chitosan does not reach the desired level of efficiency. In this work, we have employed computational methods to guide the design and development of new chitosan-based materials for adsorption of antibiotics. This study examined the functionalization of chitosan with aldehydes derivatives (figure 1), including salicylaldehyde (RCS), naphthaldehyde (RCN), and 9-anthracenecarboxaldehyde (RCA) to remove tetracycline (TC), ciprofloxacin (CPX), levofloxacin (LVX) and cephalexin (CLX) in all its forms. The interaction between antibiotics and adsorbents was analyzed using electronic structure calculations and molecular dynamics simulations. RCA is the adsorbent that shows the most efficiency in interacting with antibiotics. This is followed by RCN and last by RCS. Indeed, it appears that increasing the number of aromatic rings in the adsorbent structure improves the interaction between the adsorbents and antibiotics. We have shown that electrostatic, van der Waals, and mainly π-π interactions are the most relevant for enhancing the antibiotics adsorption.

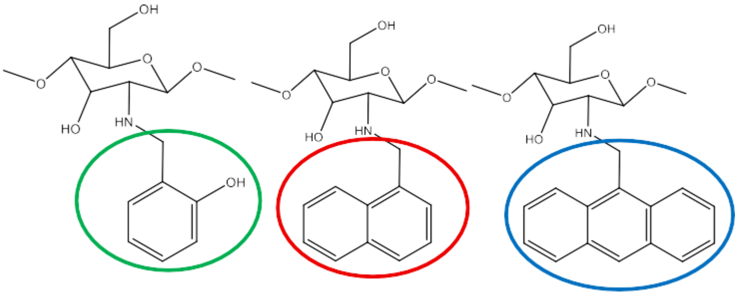

Figure 1: Structure of chitosan functionalized by salicylaldehyde (RCS) green circle in the left, naphthaldehyde (RCN) red circle in middle and 9-anthracenecarboxaldehyde (RCA) blue circle in the right.

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[1] Odonkor, S. T.; Addo, K. K. *Int J Microbiol* 2018.
[2] Das, S.; Sengupta, S. *Springer Nature Singapore* 2023, *8*, 10.
[3] Qi, X.; Tong, X.; Pan, W.; Zeng, Q.; You, S.; Shen, J. *Journal of Cleaner Production* 2021, *315*, 128221.

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SPE-UHPLC-MS/MS Method for Analysis of EU-relevant Organic Micropollutants in Portuguese Drinking Waters

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Safe and clean drinking water (DW) is a fundamental human right; however, water scarcity and poor water quality remain major global challenges [1]. In recent years, increasing scientific concern has been directed towards the widespread occurrence of micropollutants (MPs) in aquatic environments, typically detected at low concentrations ranging from ng L^{-1} to μg L^{-1} [2]. Since conventional wastewater treatment plants (WWTPs) and drinking water treatment plants (DWTPs) are generally unable to completely remove MPs [3], their presence in DW becomes more likely, potentially posing adverse effects on public health [2, 3]. Therefore, highly sensitive and precise analytical methods able to accurately determine their concentrations are crucial to deepen our knowledge on the topic, which remains insufficiently explored.

This study focuses on the optimisation, validation, and application of an offline solid-phase extraction ultra-high performance liquid-chromatography coupled to tandem mass-spectrometry (SPE-UHPLC-MS/MS) method for the determination of 24 MPs in DW, including 13 pharmaceuticals, 9 pesticides, and 2 UV-filters, listed in Decisions 2022/1307/EU and 2025/439/EU, as well as in the new Urban Wastewater Treatment Directive 2024/3019/EU. SPE optimisation led to the addition of 13.5 mg of sodium thiosulfate to a previously published protocol [4], which significantly improved the recovery rates of MPs. Method validation was successfully conducted according to international guidelines, demonstrating high analytical sensitivity, with method detection limits below 1.50 ng L^{-1}. Subsequent analysis of 50 DW samples collected from multiple regions of Portugal revealed the presence of 8 to 18 different MPs per sample. Individual quantifiable concentrations ranged from 0.13 to 131.41 ng L^{-1}, excluding some samples in which MPs such as azoxystrobin, benzotriazole, dimoxystrobin, and ipconazole were detected at concentrations exceeding the upper limits of the respective calibration curves (*i.e.*, > 116.70 ng L^{-1}). Out of the 24 target MPs, tetraconazole was the only compound not detected. Notably, to the best of our knowledge, this is the first study to both investigate and report the presence of MPs such as candesartan and imazalil in DW at a global scale, providing relevant data for worldwide MP monitoring efforts, with particular emphasis on Portugal. In addition, a preliminary human health risk assessment was conducted through the estimation of hazard quotients for the detected MPs, indicating no expected adverse effects associated with individual MPs within each sample. However, this model does not account for potential synergistic effects arising from the simultaneous presence of multiple MPs in a single sample, which may lead to an underestimation of overall health risks.

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[1] Nations, U. *The human right to water and sanitation*, 2010, 3 p.
[2] Barbosa, M. O.; Ribeiro, A. R.; Pereira, M. F. R.; Silva, A. M. T. *Analytical and Bioanalytical Chemistry*, 2016, vol. 408, p. 8355-8367.
[3] Wang, Y.; Yang, Q.; Zhang, H.; Wang, Z.; Wu, A.; Luo, Y.; Zhou, Q. *Analytica Chimica Acta*, 2024, vol. 1308, p. 342662.
[4] Gorito, A. M.; Mota, B. R.; Silva, A. M. T.; Ribeiro, A. R. L. *Journal of Chromatography A*, 2025, vol. 1756, p. 466052.

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Bisphenol-A: a hidden threat to sustainable microalgal wastewater treatment

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Bisphenol-A (BPA) is a widely used plastic additive commonly detected in wastewater (WW) due to its extensive use in consumer products and its release from microplastics [1]. As a known endocrine disruptor, BPA poses significant environmental and health risks [2]; however, it is poorly removed by conventional wastewater treatment processes [3]. This study evaluates the impact of BPA (5 and 25 mg/L, as relevant environmental concentrations) on *Chlorella vulgaris* cultivated in synthetic WW (SWW), focusing on microalgal physiology, WW bioremediation efficiency, and BPA degradation. BPA exposure led to a significant reduction in esterase activity and a dose-dependent increase in intracellular reactive oxygen species (ROS), indicating metabolic impairment and oxidative stress. Growth was notably inhibited at 25 mg/L BPA (around 44 %), resulting in reduced biomass accumulation. Despite these disruptions, photosynthetic pigment content remained stable, suggesting preservation of photochemical functionality. The presence of BPA also compromised the microalga WW polishing performance. Nitrogen and phosphorus removal efficiencies declined by up to 38 % and 34 %, respectively, and glucose uptake decreased under high BPA exposure. These functional impairments aligned with the observed physiological stress. Nevertheless, *C. vulgaris* demonstrated the ability to actively degrade BPA, achieving removal efficiencies of 34 % and 21 % for 5 and 25 mg/L, respectively, after 168 hours. Minimal degradation occurred in abiotic controls, confirming mostly the biological contribution to BPA removal. These findings highlight both the potential and limitations of microalgae-based systems for mitigating plastic additive contamination. While *C. vulgaris* exhibits tolerance and degradation capability to elevated BPA concentrations, BPA presence can significantly hinder its performance in WW treatment.

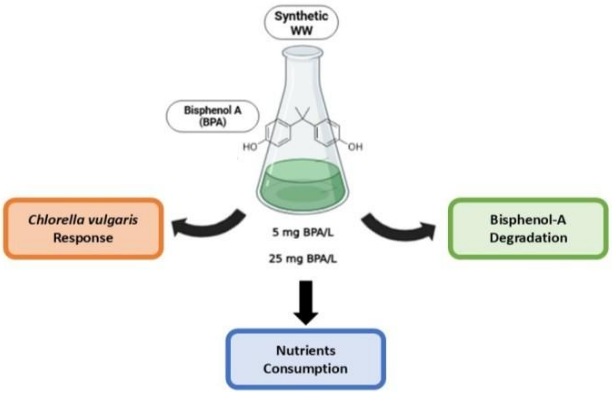

Figure 1: The potential of *Chlorella vulgaris* to bioremediate a wastewater contaminated with Bisphenol-A, at relevant environmental concentrations.

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[1] Gulnaz, O. *Journal of Applied Biological Sciences* 2009, *3*, 7.
[2] Rochester, J. R. *Reproductive Toxicology* 2013, *42*, 132–155.
[3] Yu, H. *Environmental Research* 2019, *178*, 108732

P36

Spent coffee ground-based magnetic photosensitizers for antibiotics' solar driven photocatalysis

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Antibiotic pollution constitutes an environmental and public health concern, especially due to the rising threat of antimicrobial resistance. Conventional wastewater treatment plants are often ineffective in removing pharmaceuticals such as sulfamethoxazole (SMX) and trimethoprim (TMP), which persist in aquatic environments and contribute to ecological disruption.

This research focuses on a sustainable approach for the removal of antibiotics from wastewater using magnetic solar-powered photocatalysis. For that purpose, three different protocols were tested for the production of carbon quantum dots (CQDs) from spent coffee grounds, a widely available biomass. CQDs were then integrated into titanium dioxide (TiO_2) and magnetized to facilitate recovery after photocatalysis treatment. The photocatalysts were characterized using ultraviolet-visible (UV-Vis) spectroscopy, and their performance was evaluated through solar-simulated degradation experiments. High-performance liquid chromatography with ultra-violet detection (HPLC-UV) was used to quantify antibiotic concentrations in aqueous solution before and after the photocatalyst application.

Results showed that magnetic CQDs-TiO_2 composites had compound-specific behavior. For TMP, magnetic CQDs-TiO_2 significantly enhanced degradation efficiency, as indicated by lower antibiotic concentration in aqueous solution, compared with the results obtained using magnetic TiO_2 composites (without CQDs incorporation). In contrast, magnetic CQDs-TiO_2 did not improve SMX degradation and in some cases the incorporation of CQDs in the magnetic TiO_2 even reduced the photocatalytic capacity of the composite.

This work demonstrated that magnetic CQDs-TiO_2 photocatalysts can serve as a sustainable solution for antibiotic removal from wastewater as the use of spent coffee grounds for their production supports the principles of green chemistry and circular economy. Moreover, the findings herein described underscore the importance of photosensitizer *vs.* pollutant compatibility and suggest that, while magnetic CQDs-TiO_2 are promising photocatalytic enhancers, the effectiveness of the CQDs incorporation depends on the target contaminant.

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P37

Factors influencing the ciprofloxacin stability: pH, temperature and light exposure

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Ciprofloxacin (CF), a fluoroquinolone antibiotic widely used in clinical practice, raises environmental concerns due to its persistence and its potential to induce bacterial resistance. This study aimed to evaluate the stability of CF under different conditions (pH and exposure conditions).

The antibiotic solutions were prepared with a concentration of 5 mg/L at pH 4, 7.4 and 10, and analyzed by high-performance liquid chromatography (HPLC). Samples were subjected to cold, room temperature with light and room temperature in absence of light over 27 days.

Results showed that CF is more stable under cold conditions and protected from light, with minimal variations in concentration for all the pH values considered. In contrast, significant degradation was observed in the samples exposed to light, with a reduction in concentration of 13%, 51% and 49% after 27 days for pH 4, 7.4 and 10, respectively. Thus, these results demonstrate that degradation was more obvious at pH 7.4 and 10 under light exposure.

These findings suggest that CF stability strongly depends on environmental conditions, which may explain its persistence in aquatic environments with low light and lower temperatures. Such persistence may contribute to the spread of microbial resistance, posing a risk to public health and ecosystems. This reinforces the importance of environmental monitoring and appropriate management of antibiotic-containing waste.

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P38

Removal of pharmaceuticals, consumer products and pesticides in a wastewater treatment plant in southern Madrid: a case study.

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The occurence and fate of pharmaceuticals and other anthropogenic contaminants in wasterwater have become an increasing concern for the scientific community, both due to their rising presence and to the adverse and often poorly studied effect they may exert on ecosystems and human health, within the One Health framework. Among the compounds of particular relevance are cytostatics, antibiotics, and antipsychotics.

Wastewater treatment plants (WWTPs) are primarily designed to remove organic matter of human origin. Nonetheless, their efficiency in addressing the wide diversity of pharmaceuticals and emerging contaminants still requires improvement in order to comply with current regulations and to reduce the environmental dispersion of these substances. Nevertheless, technological upgrades implemented in recent years have substantially improved treatment performance.

In this study, influent and effluent water samples were collected over three consecutive days in March 2024 from a wastewater treatment plant located in southern Madrid (Spain), which is equipped with a tertiary treatment. More than 270 compounds were analysed, including pharmaceuticals from the main therapeutic groups, metabolites, personal care and cosmetic products, as well as pesticides.

Analyses were performed using a Thermo Scientific Dionex Ultimate 3000 UHPLC system coupled to a hybrid quadrupole- Orbitrap mass spectrometer (Q Exactive Focus, ThermoFisher Scientific, California, USA) equipped with a heated electrospray ionization (HESI) source.

Out of the 270 compounds analyzed, 132 were detected. Preliminary results showed a removal of the 10% in 5 compounds, between 10-50 % in 55 compounds, 50- 75% in 37 compounds, 70-90% in 15 compounds, and over 90% in 20 compounds. The highest removal rates were observed for acetaminophen, bisoprolol, caffeine, ciprofloxacin, progesterone, and testosterone, whereas butylparaben and irbesartan showed the lowest removal.

The results indicate a high removal efficiency of pharmaceuticals and other emerging contaminants in the studied WWTP. Nevertheless, the persistence of certain compounds emphasizes the need for further optimization of treatment processes. Multi target studies such as this are essential to assess WWTP performance and to identify priority substances for future monitoring campaigns.

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Detection of Sulfamethoxazole and Trimethoprim in Surface Waters of the Dão River Using HPLC-DAD

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Antibiotics are among the most widely used pharmaceuticals in human and veterinary medicine. Their extensive use and improper disposal have led to their widespread occurrence in aquatic environments, where they pose risks to ecosystems and may contribute to the global threat of antimicrobial resistance. This study aimed to evaluate the presence of selected antibiotics in surface water from the Dão River, a regionally important water body in central Portugal, and to optimize an analytical methodology for their detection and quantification.

Water samples were collected at the Ferreirós do Dão river beach, in Spring, and two antibiotics—sulfamethoxazole and trimethoprim—were selected for analysis based on regional prescription data provided by INFARMED (Portuguese National Authority of Medicines and Health Products). Solid-phase extraction (SPE) was used to concentrate the analytes, and high-performance liquid chromatography with diode array detection (HPLC-DAD) was employed for quantification.

The analytical method was developed and validated following international guidelines. Calibration curves were obtained for both antibiotics within the range of 0.1–4.0 mg/L, with excellent linearity ($R^2 = 0.9994$ for trimethoprim and $R^2 = 0.9999$ for sulfamethoxazole). The detection limits (LOD) were 0.1886 mg/L for trimethoprim and 0.0606 mg/L for sulfamethoxazole. The quantification limits (LOQ) were 0.5716 mg/L and 0.1836 mg/L, respectively.

The results confirmed the presence of trace levels of both antibiotics in the river water samples, raising concerns about the environmental persistence of these substances and their potential ecological and public health implications. While the detected concentrations were low, the occurrence itself suggests continuous input into the river system, likely due to human usage and incomplete removal in wastewater treatment plants.

This study represents a preliminary contribution to a broader research project led by the Polytechnic Institute of Viseu, aiming to assess the environmental risk of pharmaceutical contaminants in surface waters across the Dão River basin. The findings highlight the importance of continuous monitoring and the need for improved legislation regarding pharmaceuticals in the environment, which are still not included in the EU's list of priority pollutants.

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Maria Cristina Rulli


Paolo D'Odorico

[2] The team of Zhiguo He (Zhejiang University, China)

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Zhiguo He

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Qiuhua Liang (Loughborough University, UK) and his team

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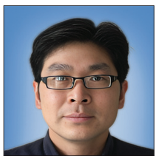
Qiuhua Liang

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Groundwater Prize

Chunmiao Zheng (EIT, Ningbo, China) and his team

for powerful modelling tools to understand groundwater processes and manage groundwater resources under diverse eco-hydrological and climatic conditions, considering environmental and socioeconomic factors at local and national scales.


Chunmiao Zheng

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Alternative Water Resources Prize

Virender K. Sharma (Texas A&M University, USA) and his team

for the effective removal of antibiotics and pharmaceuticals from wastewater through advanced oxidative processes by activated ferrate, which work at high, even enhanced, efficiency in water containing commonly occurring natural organic matter. Team members include: Ching-Hua Huang, Chetan Jinadatha and Radek Zbořil.


Virender K. Sharma

Water Management & Protection Prize

Water Management & Protection Prize

Joseph Hun-wei Lee (Macau University of Science & Technology, China)

for developing unique and highly effective hydro-environmental modelling systems for the sustainable water management of smart cities.


Joseph Hun-wei Lee

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