

BOOK OF ABSTRACTS

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

20-21 October 2025

University of Aveiro, Portugal



Title

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

Authors

Hugo Rocha Damià Barceló Goreti Pereira Vânia Calisto

Support

Electronics

Support Detail

PDF

Edition

1st Edition

Editor

Sociedade Portuguesa de Química

Graphic Design

Hugo Rocha

Book Assembly

6th ICRAPHE Organizing committee

ISBN

978-989-8124-48-7

ISBN 978-989-8124-48-7



This book was produced from works submitted directly by the authors. Only minor editorial changes were made, which in no way altered the scientific content. The final print template was established for the 6th International Conference on Risk Assessment of Pharmaceuticals in the Environment in accordance with the standards publicly disclosed in the event announcements. The authors are responsible for the scientific content.

Committees

Organizing Committee

Vânia Calisto (University of Aveiro) - Chair

Damià Barceló (University of Almería) - Co-Chair

Goreti Pereira (University of Aveiro)

Ângela Almeida (University of Aveiro)

Diana Lima (Health School, Polytechnic University of Coimbra)

Érika Sousa (University of Aveiro)

Guilherme Pinto (University of Aveiro)

Hugo Rocha (University of Aveiro)

Rita Gouveia (University of Aveiro)

Valentina Silva (University of Aveiro)

Scientific Committee

Vânia Calisto (Universidade de Aveiro, Portugal) - Chair

Damià Barceló (Universidad de Almería, Spain) - Co-Chair

Barbara Kasprzyk-Hordern (University of Bath, UK)

Cristina Delerue-Matos (Instituto Superior de Engenharia do Porto, Portugal)

Diana Aga (University at Buffalo, USA)

Gianluca Li Puma (Università degli Studi di Palermo, Italy)

Giuliana Bianco (Università della Basilicata, Italy)

Marcelo Giovanela (Universidade de Caxias do Sul, Brasil)

Marta Otero (Universidad de Léon, Spain)

Paola Verlicchi (Università degli Studi di Ferrara, Italy)

Rosa Freitas (Universidade de Aveiro, Portugal)

Rudolf Schneider (Bundesanstalt für Materialforschung und -prüfung (BAM), Germany)

Susana Loureiro (Universidade de Aveiro, Portugal)

Teresa Rocha Santos (Universidade de Aveiro, Portugal)

Secretary

Cristina Campos (SPQ)

Leonardo Mendes (SPQ)

Institutional Support













Sponsors













INDEX

Congress Information 2 Scientific Program 3 List of Communications 7 Abstracts 16 Plenary Lectures 17 Keynotes Lectures 21 Oral Communications 26 Poster Communications 53 List of Participants 93	Welcome Message	1
List of Communications 7 Abstracts 16 Plenary Lectures 17 Keynotes Lectures 21 Oral Communications 26 Poster Communications 53	Congress Information	2
Abstracts	Scientific Program	3
Plenary Lectures	List of Communications	7
Keynotes Lectures 21 Oral Communications 26 Poster Communications 53	Abstracts	16
Oral Communications	Plenary Lectures	17
Poster Communications53	Keynotes Lectures	21
	Oral Communications	26
List of Participants93	Poster Communications	53
	List of Participants	93

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!

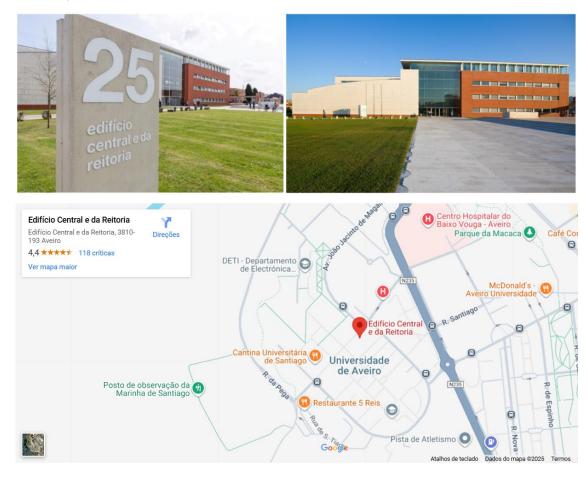
The Organizing Committee

1

Congress Information

Conference Venue

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



Scientific Program

MONDAY 20 OCTOBER 2025

8:30 Registration

9:00 Welcome Ceremony

SESSION 1 | Chair: Diana Aga

9:20 PL1 | Advances and Challenges in Molecularly Imprinted Electrochemical Sensors for Environmental Applications

Sibel A. Ozkan, Ankara University

10:10 OC1 | Monitoring Endocrine-Disrupting Pharmaceuticals in Belgian Tap and Bottled Water: Insights from the AquaGlance Study

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

11:20 KN1 | How can antibodies help us in the risk assessment of pharmaceuticals in the environment?

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

12:35 The Prince Sultan Bin Abdulaziz International Prize for Water

12:50 Lunch

SESSION 3 | Chair: Diana Lima

14:00 PL2 | Intensification of Advanced Oxidation Processes in Multi-Scale Reactors for the Removal of Pharmaceuticals Residues in Water

Gianluca Li Puma, University of Palermo

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

Pedro M. C. Matias, Universidade de Coimbra

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

Cigdem Kalkan Aktan, Marmara University

15:20 OC9 | Efficient Removal of 17a-Ethinylestradiol from Water Using Silica-Based Adsorbents: Impact of Organic Functionalities and Water Matrices

Tiago F. T. Morais, Universidade De Aveiro

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

Angelica R. Zizzamia, University of Basilicata

15:50 OC11 | Effect of diclofenac on wastewater treatment with aerobic granular sludge: performance and biopolymer production

Joana Batista, NOVA FCT

16:05 Coffee-Break

16:30 Poster Session 1

SESSION 4 | Chair: Rudolf J. Schneider

17:00 KN2 | Electrobiomediation of pharmaceuticals in urban and industrial wastewater: the METFILTER® modular solution

Abraham Esteve-Núñez, University of Alcalá, IMDEA Agua

17:30 OC12 | Sustainable Fixed-Bed Adsorption of Antibiotics from Wastewater Using Regenerable Biochar Derived from Brewery Residues

Érika M. L. Sousa, University of Aveiro

17:45 OC13 | Efficiency of the Asian Clam in Removing Pharmaceuticals from Wastewater

André Pereira, University of Coimbra

18:00 OC14 | Titanium Dioxide Nanoparticles-Integrated with MIP for Highly Selective Electrochemical Cefepime Sensing in Environmental Samples

Ahmet Cetinkaya, Ankara University

18:30 Social Programme and Conference Dinner

Moliceiro Boat Ride and Dinner at Restaurant Solar do Bacalhau

TUESDAY 21 OCTOBER 2025

8:30 Registration

SESSION 5 | Chair: Susana Loureiro

9:00 PL3 | Pharmaceutical Pollution Meets Climate Pressure-. Aquatic Ecosystems at a Crossroads

Rosa Freitas, University of Aveiro

9:50 OC15 | Assessment of the ecotoxicological effects of levamisole, an antiparasitic drug used off-label in aquaculture

Alyson R. Ribeiro, Federal University of Minas Gerais

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

10:20 OC17 | Hidden costs of beauty: An in vitro study on the ecotoxicological impacts of Parabens and Ultraviolet Filters on bioindicator species Mytilus galloprovincialis

Diana Bordalo, Universidade de Aveiro

10:35 Coffee-break

11:05 Poster Session 2

SESSION 6 | Chair: Rosa Freitas

11:35 KN3 | Assessing the Environmental Impact of Veterinary Pharmaceuticals

Lucia De Marchi, University of Pisa

12:05 OC18 | Microplastics as Vector for Pharmaceuticals: Analytical Challenges and

Ecotoxicological Risks in Aquatic Systems

Ana L. Patrício Silva, Universidade de Aveiro

12:20 OC19 | New Approach Methodologies predict pharmaceutical pollution

Emma Rowan, Dublin City University

12:35 Lunch

SESSION 7 | Chair: Giuliana Bianco

14:00 KN4 | Exploring the role of enantioselectivity in environmental process

Ana Rita Lado Ribeiro, FEUP

14:30 OC20 | Development and Validation of an Analytical Method for Veterinary Antibiotics in Wastewater Using SPE-HPLC

Isabel Brás, IPV-ESTGV

14:45 OC21 | Reuse of reclaimed water (EU 2020/741) and release of treated effluent (EU 2024/3019) – The selection of priority CECs for monitoring plans

Paola Verlicchi, University of Ferrara

15:00 OC22 | Advanced Environmental Control Technologies: Integrated Analytical Solutions for Emerging Contaminants (**Sponsor** | **Unicam Sistemas Analíticos Lda**)

Daniel Ettlin, Unicam Sistemas Analíticos Lda

15:20 Coffee-break

SESSION 8 | Chair: Susana Loureiro & Maria Pavlaki

15:50 OC23 | Boosting the reduction of the environmental impact of pharmaceutical products throughout their entire life cycle

Chiara Ilgrande, AIMPLAS – Technological Institute of Plastics

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

Robert Peeling, Britest Ltd

16:30 OC25 | Modelling the Emissions of Pharmaceuticals to the Environment

Hongyan Chen, UK Centre for Ecology & Hydrology

16:50 OC26 | Hazard Assessment of Pharmaceuticals and their Production Process: Diclofenac as a case study

Carolina Machado, Universidade de Aveiro

17:10 Closing Ceremony and Awards

List of Communications

Plenary Lectures

PL1. Sibel A. Ozkan

Advances and Challenges in Molecularly Imprinted Electrochemical Sensors for Environmental Applications

PL2. Gianluca Li Puma

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

PL3. Rosa Freitas

Pharmaceutical Pollution Meets Climate Pressure: Aquatic Ecosystems at a Crossroads

Keynote Lectures

KN1. Rudolf J. Schneider

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

KN2. Abraham Esteve-Núñez

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

KN3. Lucia de Marchi

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

KN4. Ana Rita Lado Ribeiro

Exploring the role of enantioselectivity in environmental processes

Oral Communications

OC1. Tess Goessens

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

OC2. Flavia Melati Chiappara

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

OC3. Vanessa Maybruck

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

OC4. Diana S. Aga

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

OC5. Merve Yence

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

OC6. Farah Elbaghathi

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

OC7. Pedro M. C. Matias

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

OC8. Cigdem Kalkan Aktan

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

OC9. Tiago Morais

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

OC10. Angelica R. Zizzamia

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

OC11. Joana Batista

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

OC12. Érika M. L. Sousa

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

OC13. André Pereira

Efficiency of the Asian Clam in Removing Pharmaceuticals from Wastewater

OC14. Ahmet Cetinkaya

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

OC15. Alyson R. Ribeiro

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

OC16. Sofia C. Walzer

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

OC17. Diana Bordalo

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

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

OC20. Isabel Brás

Development and Validation of an Analytical Method for Veterinary Antibiotics in Wastewater using SPE-HPLC

OC21. Paola Verlicchi

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

OC22. Daniel Ettlin (Sponsor)

Advanced Environmental Control Technologies: Integrated Analytical Solutions for Emerging Contaminants

OC23. Chiara Ilgrande

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

OC24. Robert Peeling

The Need for an Early-Stage Sustainability Assessment Methodology

OC25. Hongyan Chen

Modelling the Emissions of Pharmaceuticals to the Environment

OC26. Carolina Machado

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

Poster Communications

P1. Beatriz Camarneiro

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

P2. Filomena Lelario

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

P3. Filomena Lelario

Evaluation of electrochemical degradation using a platinum anode for venlafaxine removal

P4. Joanna Dołżonek

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

P5. Magda Caban

Miniaturization of Ecotoxicological Tests and Their Application to Assess the Toxicity of β -Blockers Towards Cyanobacterium Mycrocystis aeruginosa

P6. Fernanda Rodrigues

TiO₂ photocatalyst supported on superparamagnetic silica aerogel for sunlight-activated removal of pharmaceuticals from wastewaters

P7. Anna Białk-Bielińska

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

P8. Ensar Piskin

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

P9. Beyza Unal

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

P10. Ana Rita Loureiro

Development of Copper Nanomaterials as Nanozymes for Advanced Water Treatment

P11. Ângela Almeida

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

P12. Rita Gouveia

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

P13. Maria Fernanda Nogueira

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

P14. Valentina Silva

Application of magnetic TiO2/Carbon Quantum Dots for efficient removal of antibiotics from water

P15. Hugo F. Rocha

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

P16. Rudolf J. Schneider

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

P17. Angelica R. Zizzamia

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

P18. Grazia Accoto

Chemical Substances Watch List: A Tool for Monitoring and Prevention

P19. Emma Rowan

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

P20. Flavia Melati Chiappara

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

P21. Guilherme F. Pinto

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

P22. Diana Bordalo

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

P23. Lucélia Hoehne

Pistia stratiotes L. (Araceae) exposed to amoxicillin: implications for ecotoxicological risk assessment in aquatic systems

P24. Zélia Barbosa

Green synthesis of silver and copper QDs as promising radiopharmaceuticals

P25. Igor E. Oliveira

Synthesis of nadifloxacin derivatives for further ecotoxicological studies

P26. Fabiana Y. M. Vieira

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

P27. Leonor R. Barroca

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

P28. Beatriz Suordem

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

P29. Joaquín A. Marrero

Selection of ofloxacin-degrading microorganisms from activated sludge microbiota

P30. Maria D. Pavlaki

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

P31. Alexandre van Heerden

Selective antibacterial effects of fluoroquinolones on wastewater bacteria

P32. Beatriz Valadares

Incorporation of TiO₂/CQDs into polymeric fibers for the photodegradation of amoxicillin in water

P33. Joana F. M. Sousa

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

P34. Inês M. Quintela

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

P35. Paulo M. S. Sousa

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

P36. Carla Patrícia Silva

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

P37. Ana Paula Fonseca

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

P38. Yolanda Valcárcel

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

P39. Isabel Brás

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

Abstracts

Plenary Lectures



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

20 - 21 October, 2025 - Aveiro

PL1

Advances and Challenges in Molecularly Imprinted Electrochemical Sensors for Environmental Applications

Sibel A. Ozkan1*

¹Ankara 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.



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

20 - 21 October, 2025 - Aveiro

PL2

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

Gianluca Li Puma^{1*}

¹Environmental Nanocatalysis & Photoreaction Engineering, Department of Engineering, University of Palermo (UNIPA), 90128 Palermo, Italy

*ginaluca.lipuma@unipa.it

Advanced oxidation processes (AOP), such photolysis, UV-H₂O₂, 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/H₂O₂ 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/H₂O₂ 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.



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

20 - 21 October, 2025 - Aveiro

PL3

Pharmaceutical Pollution Meets Climate Pressure: Aquatic Ecosystems at a Crossroads

Rosa Freitas1*

¹Department 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 speciesspecific 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



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

20 - 21 October, 2025 - Aveiro

KN1

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

Rudolf J. Schneider^{1,*}

¹BAM 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



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

20 - 21 October, 2025 - Aveiro

KN2

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

Abraham Esteve-Núñez^{1,2,3*}

¹Universidad de Alcalá, Madrid, Spain ²IMDEA WATER, Madrid, Spain ³METfilter, Madrid, Spain *abraham.esteve@uah.es

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.



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

20 - 21 October, 2025 - Aveiro

KN3

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

Lucia De Marchi1*

¹Department of Veterinary Science, Università di Pisa, Via Livornese snc 56122 San Piero a Grado Pisa, Italy *lucia.demarchi@unipi.it

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

Communication, Dissemination and Exploitation

Population

Organism

Organ

Tissue

Cell

Physioidics
Antinicipala
activity
Antinicipala
Activity
Nature-based

Figure 1:Graphical representation of the SOURCE project impact

responses—even at concentrations commonly detected in aquatic environments [7,8].

these challenges. Given 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 Healthaligned 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.



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

20 - 21 October, 2025 - Aveiro

KN4

Exploring the role of enantioselectivity in environmental processes

Ana Rita Lado Ribeiro^{1,2,*}

¹LSRE-LCM – Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

²ALICE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

*ritalado@fe.up.pt

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.

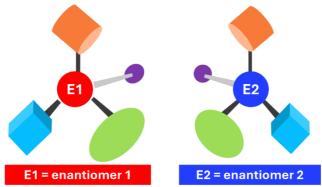


Figure 1: Representation of the three-dimensional asymmetry of the enantiomers of a chiral compound.

Acknowledgements: Funded by the European Union (ERC, ERA-ARE, project number 101039270). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council Executive Agency. Neither the European Union nor the granting authority can be held responsible for them. This research was also supported by: project 2022.02842.PTDC – STAR - STereoselective environmental processes in Antibiotics: role for Resistance, with DOI 10.54499/2022.02842.PTDC (https://doi.org/10.54499/2022.02842.PTDC), UID/50020 of LSRE-LCM - Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials - funded by Fundação para a Ciência e a Tecnologia, I.P. /MCTES through national funds; and ALiCE - LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020). ARLR acknowledges the support from FCT funding under the Scientific Employment Stimulus - Individual Call 2022.00184.CEECIND/CP1733/CT0001 (DOI: 10.54499/2022.00184.CEECIND/CP1733/CT0001).

[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



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

20 - 21 October, 2025 - Aveiro

OC1

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

T. Goessens^{1*}, A. Chen¹, N. N. Truong¹, S. De Saeger^{1,2}, L. Vanhaecke^{3,4} and M. De Boevre¹

¹Centre of Excellence in Mycotoxicology and Public Health, Faculty of Pharmaceutical Sciences, Ghent University, Ghent Belgium

²Department of Biotechnology and Food Technology, Faculty of Science, University of Johannesburg, Johannesburg, South-Africa

³Laboratory of Integrative Metabolomics, Faculty of Veterinary Medicine, Ghent University, Merelbeke, Belgium

⁴Queen's University Belfast, School of Biological Sciences, Institute for Global Food Security, Chlorine Gardens 19, BT9-5DL Belfast, Northern Ireland, United Kingdom *tess.goessens@ugent.be

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 ($C_{max} = 60.2 \text{ ng/L}$). 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.

Acknowledgements: This research was supported by the Research Foundation – Flanders (FWO, grant no. 1204324N), the European Research Council (ERC, HUMYCO, grant no. 946192), and the Industrial Research Fund of Ghent University (IOF, F2021/IOF-Equip/014).



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

20 - 21 October, 2025 - Aveiro

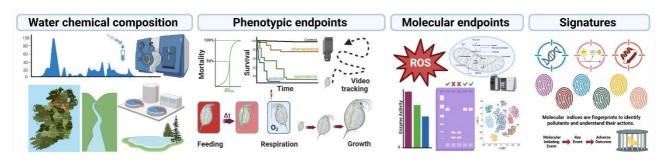
OC2

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

<u>Flavia Melati Chiappara</u>^{1*}, Izabela Malgorzata Antepowicz¹, Maria Eleni Tsioli¹, Anne Leung¹, Emma Rowan¹, Konstantinos Grintzalis¹

¹School of Biotechnology, Dublin City University, Ireland *flavia.melatichiappara2@mail.dcu.ie

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.





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

20 - 21 October, 2025 - Aveiro

OC4

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

Vanessa Maybruck^{1,2,*}, Cresten Mansfeldt^{1,3}

¹University of Colorado Boulder, Environmental Engineering Program, 4001 Discovery Drive, Boulder, Colorado 80303, United States of America

²University of Colorado Boulder, BioFrontiers Institute, 3415 Colorado Avenue, Boulder, Colorado 80303, United States of America.

³University of Colorado Boulder, Department of Civil, Environmental & Architectural Engineering, 1111 Engineering Drive, Boulder, Colorado 80309, United States of America. *vanessa.maybruck@colorado.edu

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 nontarget 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.

Acknowledgements: Thanks to Jamie Akens, Cole Sigmon, and the Boulder Water Resource Recovery Facility for providing the MLSS. This work was supported in part by the Interdisciplinary Quantitative Biology (IQ Biology) PhD program at the BioFrontiers Institute, University of Colorado Boulder, and the National Science Foundation NRT Integrated Data Science Fellowship (award 2022138). This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE 2040434. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

[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.



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

20 - 21 October, 2025 - Aveiro

OC4

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

Diana S. Aga1*

¹Henry Woodburn Professor of Chemistry, Department of Chemistry University at Buffalo, The State
University of New York, NY USA
*dianaaga@buffalo.edu

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.





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

20 - 21 October, 2025 - Aveiro

OC5

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

Merve Yence^{1*}, Ahmet Cetinkaya^{2,3}, Mehmet Gokhan Caglayan⁴, Sibel A. Ozkan⁴

¹Lokman Hekim University, Faculty of Pharmacy, Department of Analytical Chemistry, 06510, Ankara, Türkiye.

²University of Health Sciences, Gulhane Faculty of Pharmacy, Department of Analytical Chemistry, 06018, Ankara, Türkiye

³Hacettepe University, Faculty of Pharmacy, Department of Analytical Chemistry, 06230, Ankara, Türkiye ⁴Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, 06560, Ankara, Türkiye *merve.yence@lokmanhekim.edu.tr

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.



20 - 21 October, 2025 - Aveiro

OC6

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

<u>Farah Elbaghathi^{1,2*}</u>, Ensar Piskin^{1,2}, Ahmet Cetinkaya^{3,4}, Aytekin Uzunoglu⁵, Esen Bellur Atici^{6,7}, Sibel A. Ozkan¹, Burcu Dogan-Topal¹

¹Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

²Ankara University, Graduate School of Health Sciences, Ankara, Türkiye

³University of Health Sciences, Gülhane Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

⁴Hacettepe University Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

⁵Istanbul Technical University, Faculty of Chemical and Metallurgical Engineering, Department of

Metallurgical and Materials Engineering, İstanbul, Türkiye

⁶DEVA Holding A.S., R&D Center, Tekirdağ, Türkiye

⁷Gebze Technical University, Department of Chemistry, Kocaeli, Türkiye

*farahsoliman9490@gmail.com

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.

$$O$$
 O NH O NH_2

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



20 - 21 October, 2025 - Aveiro

OC7

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

Pedro M. C. Matias^{1,*}, Talles B. Costa^{1,2}, Derval S. Rosa², Dina M. B. Murtinho¹, Artur J. M. Valente¹

¹CQC-IMS, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal.

²CECS, Federal University of ABC, 09280-560 Santo André, SP, Brazil

*petermatias1998@gmail.com

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 iminelinked 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.

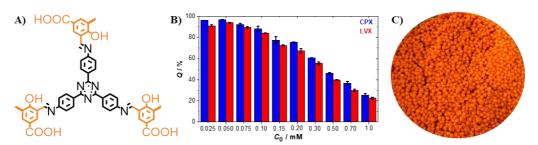


Figure 1: A) Chemical structure of IT-POP; B) Effect of the initial concentration on the removal efficiencies of CPX and LVX by IT-POP; C) Photograph of IT-POP-containing starch-alginate beads.

Acknowledgements: To Coimbra Chemistry Centre (CQC-IMS), supported by Fundação para a Ciência e a Tecnologia (FCT, Portugal) through the programs UIDB/00313/2025 & UIDP/00313/2025. Pedro M. C. Matias also thanks FCT (Portugal) for the PhD Grant 2022.12425.BD (financed by Portuguese State Budget and cofinanced by PDQI program). This study was also financed, in part, by FAPESP (Brazil) through processes #2022/11133-0, #2023/11783-8 and #2020/13703-3.

^[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.



20 - 21 October, 2025 - Aveiro

OC8

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

<u>Cigdem Kalkan Aktan^{1,2*}</u>, Erkan Sahinkaya¹, Giuliana Bianco³, Donatella Caniani², Angela Di Capua³, Francesco Di Capua²,

¹Department of Environmental Engineering, Marmara University, 34722 Goztepe, Istanbul, Turkey University ² Department of Engineering, University of Basilicata, Via dell'Ateneo Lucano 10, 85100 Potenza, Italy

*cigdemkalkan@marmara.edu.tr

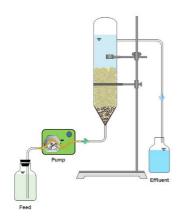
This study investigates the co-removal efficiency of nitrate and five widely used pharmaceutical compounds triclosan, ibuprofen, carbamazepine, naproxen, and diclofenac in a lab-scale autotrophic denitrification column bioreactor. Nitrate concentrations (5–30 mg/L) and pharmaceuticals (constant at 5 μ g/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.



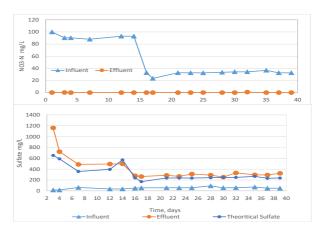


Figure 1: Schematic view of reactor

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).

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

³ Department of Basic and Applied Sciences, University of Basilicata, Via dell'Ateneo Lucano 10, 85100 Potenza, Italy



20 - 21 October, 2025 - Aveiro

OC9

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

<u>Tiago Morais</u>^{1,2,*}, Diogo Pereira³, Geraldine Sequera¹, Ana C. Moreira¹, Marina Ilkaeva^{1,4}, Luís Mafra¹, Mariana Sardo¹, Vânia Calisto¹, Mirtha A. O. Lourenço¹

- ¹ CICECO Instituto de Materiais de Aveiro, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal
- Department of Chemistry, University of Iceland, Science Institute, Dunhaga 3, 107 Reykjavik, Iceland
 CESAM, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193
 Aveiro, Portugal
- ⁴ Department of Chemical and Environmental Engineering, University of Oviedo, Av. Julián Clavería 8, 33006 Oviedo, Spain *tiagomorais@ua.pt

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 µg 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 vinvl-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.

Acknowledgements: This work was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MEC (PIDDAC). The authors also acknowledge financial support to CESAM by FCT/MCTES (UIDP/ 50017/2020+ UIDB/50017/2020+ LA/P/0094/2020), through national funds. The NMR spectrometers are part of the National NMR Network (PTNMR) and are partially supported by Infrastructure Project 022161 (cofinanced by FEDER through COMPETE 2020, POCI and PORL and FCT through PIDDAC). This work has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant Agreement 865974). FCT is also acknowledged by D.P. for a Ph.D. Studentship (2020.05389. BD), M.I., M.A.O.L. and M.S. for Researcher positions (CEECIND/00546/2018, CEECIND/01158/2021 and CEECIND/00056/2020, respectively). M.A.O.L further acknowledges the funding from the European Union's Horizon Europe research and innovation programme (ERA-PF grant agreement No 101090287). MI also acknowledges Spanish Ministry of Science, Innovation and Universities for the "Beatriz Galindo" Scholarship (MU-23-BG22/00145).



20 - 21 October, 2025 - Aveiro

OC10

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

A.R. Zizzamia1*, Â. Almeida2, M. V. Gil3, F. Lelario1, V. Calisto2

¹University of Basilicata, 85100 Potenza, Italy
²Department of Chemistry & CESAM, University of Aveiro, 3810-193 Aveiro, Portugal
³Instituto de Ciencia y Tecnología del Carbono, INCAR (CSIC), Oviedo, Spain
*angelicarebecca.zizzamia@unibas.it

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, reentering 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.

Acknowledgements: This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P. under the project/grant UID/50006 + LA/P/0094/2020. The authors also thank Faustino Microcervejeira, Lda. (Aveiro, Portugal) and its head brewer Gonçalo Faustino for kindly providing the brewing residues used in this work.

- [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.



20 - 21 October, 2025 - Aveiro

OC11

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

Joana Batista^{1,2}, Federica Perbellini^{1,2}, Maria Reis^{1,2}, Nídia Lourenço^{1,2*}

¹Associate Laboratory i4HB–Institute for Health and Bioeconomy, Department of Chemistry, NOVA University Lisbon, 2829-516 Caparica, Portugal ²UCIBIO – Applied Molecular Biosciences Unit, Department of Chemistry, NOVA School of Science and Technology, NOVA University Lisbon, 2829-516 Caparica, Portugal

*nidia.lourenco@fct.unl.pt

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 μ g 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.

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-¹d-1, acetate was totally consumed at the end of the nonaerated reaction stage, and for 25.6 gCODL-1d-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 accumulating organisms (PAO) was polyphosphate negatively affected by DCF. Also, regardless of the Csource 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

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

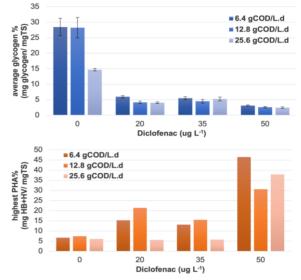


Figure 1: Effect of DCF concentration on glycogen and PHA content (%m/m).

AGS physical robustness, the granules' settle ability was not affected by either DCF or C,N,P concentrations. 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.

Acknowledgements: This work was financed by national funds from FCT - Fundação para a Ciência e a Tecnologia, I.P., in the scope of the project UIDP/04378/2020 and UIDB/04378/2020 of the Research Unit on Applied Molecular Biosciences - UCIBIO, and the project LA/P/0140/2020 of the Associate Laboratory Institute for Health and Bioeconomy - i4HB.



20 - 21 October, 2025 - Aveiro

OC12

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

<u>Érika M.L. Sousa^{1*}</u>,Marta Otero², Rita Gouveia³, Paula Quinteiro⁴, Luís A.C. Tarelho⁵, Márcia Santos⁵, María V. Gil⁶, Paula Ferreira⁷, Valdemar I. Esteves¹, Vânia Calisto¹

¹Department of Chemistry and CESAM, University of Aveiro, Portugal
²Departamento de Química y Física Aplicadas, Universidad de León, Spain
³Department of Chemistry, University of Aveiro, Portugal
⁴Department of Environment and Planning and CESAM, University of Aveiro, Portugal
⁵Department of Materials and Ceramic Engineering and CICECO, University of Aveiro, Portugal
⁶Instituto de Ciencia y Tecnología del Carbono, INCAR (CSIC), Oviedo, Spain
⁷Department of Materials & Ceramic Engineering and CICECO, University of Aveiro, Portugal
*erikamsousa@ua.pt

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 m² g⁻¹ in cycle 1 to 462 m² 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.



20 - 21 October, 2025 - Aveiro

OC13

Efficiency of the Asian Clam in Removing Pharmaceuticals from Wastewater.

Mariana Lopes¹, João Gomes², André Pereira¹, Liliana Silva¹*

¹ LAQV, REQUIMTE, Laboratory of Bromatology and Pharmacognosy, Faculty of Pharmacy, University of Coimbra, Polo III, Azinhaga de Sta Comba, 3000-548 Coimbra, Portugal
²University of Coimbra, CERES, Department of Chemical Engineering, Faculty of Sciences and Technology, Rua Sílvio Lima, Polo II, 3030-790 Coimbra, Portugal.
*Ijgsilva@ff.uc.pt

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.É.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.



20 - 21 October, 2025 - Aveiro

OC14

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

Ahmet Cetinkaya^{1,2}*, Sibel A. Ozkan³

¹University of Health Sciences, Gülhane Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

²Hacettepe University Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

³Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

*ahmet.cetinkya@yahoo.com

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 (TiO₂NPs) 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/TiO₂NPs/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.

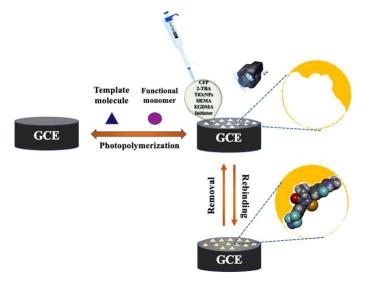


Figure 1. Schematic representation of the developed sensor

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



20 - 21 October, 2025 - Aveiro

OC15

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

Caroline P. Ribeiro de Souza¹, Jose A. Casas², Juan A. Zazo Martinez², <u>Alyson R. Ribeiro^{1,2*}</u>

¹Veterinary School, Federal University of Minas Gerais, 31270-901 Belo Horizonte, Minas Gerais, Brazil.

²Chemical Engineering, Universidad Autónoma de Madrid, 28049 Madrid, Spain.

*alysonrogerio@ufmq.br

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).

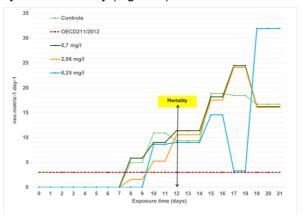


Figure 1: 21 days reproductive performance of *D. similis* exposed to Levamisole

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.



20 - 21 October, 2025 - Aveiro

OC16

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

Sofia C. Walzer^{1,*}, Imke M. Böök¹, Andreia Farinha¹, Louis Simon¹, Micaela S. S. Justo¹, Susana Carvalho¹

¹Division of Biological and Environmental Science and Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia
*sofia.walzer@kaust.edu.sa

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.

Acknowledgements: Vijayalaxmi Dasari, Fern Lyne-Temple, Huajing Yan, Gage A. Mele, Vasco P. Oliveira, Farhat Un Nisa N. Bajwa, Lorenzo Raeli, Biodiversity and Ecosystem Management Lab, Coastal and Marine Resources Core Lab.

- [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



20 - 21 October, 2025 - Aveiro

OC17

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

Diana Bordalo^{1*}, Amadeu M.V.M Soares¹, Inna Sokolova^{2,3}, Carlo Pretti^{4,5}, Rosa Freitas¹

¹Department of Biology & CESAM, University of Aveiro, 3810-193 Aveiro, Portugal

²Department of Marine Biology, Institute for Biological Sciences, University of Rostock, Rostock, Germany

³Department of Maritime Systems, Interdisciplinary Faculty, University of Rostock, Rostock, Germany

⁴Department of Veterinary Sciences, University of Pisa, Viale delle Piagge 2, 56124 Pisa, Italy

⁵Interuniversity Consortium of Marine Biology of Leghorn "G. Bacci", 57128 Livorno, Italy

*dianabordalo@ua.pt

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.

Acknowledgements: Diana Bordalo was supported by Ph.D. grant (2023.01230.BD) from the National Funds through the Portuguese Science Foundation (Fundação para a Ciência e a Tecnologia, FCT). This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020. Financial support was also provided by ACTNOW project funded by the European Union's Horizon Europe research and innovation programme under grant agreement no. 101060072.



20 - 21 October, 2025 - Aveiro

OC18

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

Ana L. Patrício Silva1*, Teresa Rocha-Santos2

¹ Centre for Environmental and Marine Studies (CESAM) and Department of Biology, University of Aveiro,
Aveiro 3810-193, Portugal

²Centre for Environmental and Marine Studies (CESAM) and Department of Chemistry, University of Aveiro, Aveiro 3810-193, Portugal
*ana.luisa.silva@ua.pt

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.



20 - 21 October, 2025 - Aveiro

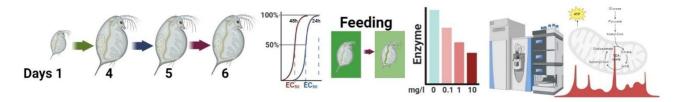
OC19

New Approach Methodologies predict pharmaceutical pollution

Emma Rowan^{1*}, Flavia Melati Chiappara¹, Izabela Malgorzata Antepowicz¹, Maria Eleni Tsioli¹, Anne Leung¹, Konstantinos Grintzalis¹

¹School of Biotechnology, Dublin City University, Ireland *emma.rowan4@mail.dcu.ie

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.





20 - 21 October, 2025 - Aveiro

OC20

Development and Validation of an Analytical Method for Veterinary Antibiotics in Wastewater Using SPE-HPLC

Isabel Brás^{1,*}, Elisabete Silva ^{1,2}

¹Polytechnic University of Viseu – ESTGV, Campus Politécnico, Repeses, 3504-510, Viseu, Portugal, CISeD Research Centre, Polytechnic University of Viseu – ESTGV, Campus Politécnico, Repeses, 3504-510, Viseu, Portugal

²LEPABE-Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto (FEUP), R. Dr. Roberto Frias S/N, 4200-465 Porto, Portugal *ipbras@estqv.ipv.pt

Veterinary antibiotics are increasingly recognized as environmental contaminants of emerging concern due to their widespread use in intensive livestock production and subsequent discharge into water bodies. Their presence in aquatic environments raises significant ecological and public health concerns, especially the proliferation of antibiotic-resistant bacteria. This study aimed to develop and validate a solid-phase extraction (SPE) and high-performance liquid chromatography (HPLC-DAD) method for the detection and quantification of three veterinary antibiotics—amoxicillin, enrofloxacin, and oxytetracycline—in wastewater matrices.

The method was developed and tested using spiked samples of distilled water, lagoon water, and pig slurry (manure). Extraction was performed with C18 SPE cartridges, and the analytes were eluted with methanol, followed by solvent evaporation and reconstitution. Chromatographic separation was achieved on a C18 column using a gradient elution program with phosphoric acid and acetonitrile as mobile phases. Detection was performed using diode array detection (DAD) at 220 nm for amoxicillin and 280 nm for enrofloxacin and oxytetracycline.

Calibration curves were prepared with mixed standards across appropriate concentration ranges: 1.7-27 mg/L for amoxicillin and 0.8-13 mg/L for the other two antibiotics. Good linearity was observed for enrofloxacin ($R^2 = 0.9936$) and oxytetracycline ($R^2 = 0.9999$), but not for amoxicillin ($R^2 = 0.9570$). Recovery rates varied significantly depending on the matrix and extraction volume, with the highest recoveries achieved for amoxicillin ($\sim 38\%$) in samples spiked at 50 ppb. The method's precision and accuracy were evaluated according to international validation guidelines, showing acceptable Z-scores for enrofloxacin and oxytetracycline, but not for amoxicillin. Precision parameters (CV%) exceeded acceptable limits in several cases, especially at higher concentrations.

While the method allowed quantification of antibiotics in fortified samples, it did not yield reliable results for real wastewater samples (pig slurry and lagoon water), likely due to matrix effects, low analyte concentrations, and instrumental issues with the HPLC system. The study highlights the analytical challenges posed by complex matrices and the importance of robust method validation for reliable environmental monitoring. Although not fully validated, the methodology provided valuable insights for future improvements in detecting veterinary antibiotics in wastewater. This work contributes to broader efforts to assess the environmental risk of pharmaceutical residues from animal husbandry and reinforces the need for continuous method development in this field.

Acknowledgements: This work was financed by National Funds through FCT - Foundation for Science and Technology, I.P., under the project Ref.^a UIDB/05583/2020. We additionally thank the Digital Services Research Center (CISeD) and the Polytechnic Institute of Viseu for the support provided.



20 - 21 October, 2025 - Aveiro

OC21

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

Paola Verlicchi^{1*}. Vittoria Grillini¹

¹Department of Engineering, University of Ferrara, Via Saragat 1 44122 Ferrara - Italy *paola.verlicchi@unife.it

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 Kow) 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, *42*9, 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



20 - 21 October, 2025 - Aveiro

OC22

Advanced Environmental Control Technologies: Integrated Analytical Solutions for Emerging Contaminants

Daniel Ettlin^{1,2*}

¹Unicam Sistemas Analíticos Lda., 1495-132 Miraflores, Portugal ²Alves Jorge, Rua da Ponte da Pedra 406, 4470-108 Gueifães Maia, Portugal *daniel.ettlin@thermounicam.pt

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 μ m down to 1 μ m. 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.

Acknowledgements: We would like to express our gratitude to the Center of Excellence of Thermo Scientific in Villebon for their valuable support and for sharing the data used in this presentation.



20 - 21 October, 2025 - Aveiro

OC23

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

Chiara Ilgrande^{1*}, Carlos Fernández Ruiz¹

¹. AIMPLAS - Technological Institute of Plas0tics, 46980 Paterna (Spain) *cilgrande@aimplas.es

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.



20 - 21 October, 2025 - Aveiro

OC24

The Need for an Early-Stage Sustainability Assessment Methodology

Robert Peeling^{1,*}, John Henderson¹

¹Britest Limited, Colony, 5 Piccadilly Place Manchester M13BR, United Kingdom

*r.p@britest.co.uk

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.

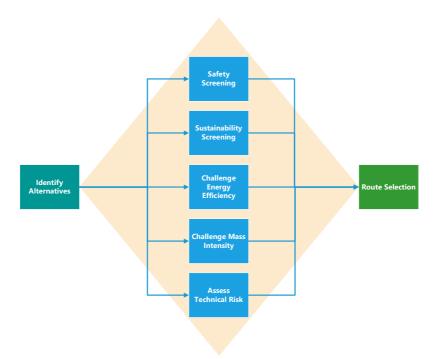


Figure 1: Overview of Methodology for Early-Stage Sustainability Assessment for Chemical and Biochemical Manufacturing Processes

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 quarantee.

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



20 - 21 October, 2025 - Aveiro

OC25

Modelling the Emissions of Pharmaceuticals to the Environment

H Chen^{1*} and S Harrison¹

¹UK Centre for Ecology and Hydrology

*honche@ceh.ac.uk

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.

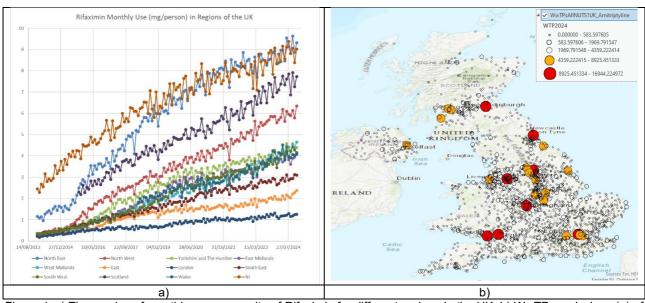


Figure 1: a) Time series of monthly use per capita of Rifaximin for different regions in the UK; b) WwTPs emissions (g) of Amitriptyline [3] in 2024.

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



20 - 21 October, 2025 - Aveiro

OC26

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

Carolina Machado^{1*}, Maria D. Pavlaki¹, Iria Naveira-Souto², Madalena Vieira¹, Filippo Fabbri³, Cicely May Warne³, Fábio Yu Chen¹, Patrícia V. Silva¹, Amadeu M.V.M. Soares¹, Georg Guebitz³, Elisabet Rosell-Vives², Susana Loureiro¹

¹CESAM & Department of Biology, University of Aveiro, Campus Universitário de Santiago, Aveiro, Portugal ²Pharmaceutical Innovation, Laboratorio Reig Jofre, S.A. Gran Capità, 10. Sant Joan Despí 08970, Barcelona, Spain

³Institute of Environmental Biotechnology, University of Natural Resources and Life Sciences Vienna Konrad-Lorenz-Strasse 20, 3430 Tulln an der Donau, Austria. *carolina02@ua.pt

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.

Acknowledgements: This publication has received funding from the European Union's Horizon Europe Framework Programme (HORIZON) under grant agreement No 101057668. CESAM affiliated co-authors acknowledge Fundação para a Ciência e a Tecnologia, Ministério da Ciência, Tecnologia e Ensino Superior (FCT/MCTES), Portugal, for the financial support to CESAM under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020) and MDP under the Scientific Employment Stimulus - Individual Call (CEEC Individual) - 2023.06417.CEECIND/CP2849/CT0014 (https://doi.org/10.54499/2023.06417.CEECIND/CP2840/CT0014), through national funds.

[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



20 - 21 October, 2025 - Aveiro

Р1

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

Beatriz Camarneiro^{1*}, Ângela Almeida², Vânia Calisto²

¹Chemistry Department, University of Aveiro, 3810-193 Aveiro, Portugal
² Chemistry Department & CESAM, University of Aveiro, 3810-193 Aveiro, Portugal
*beatriz.antunes@ua.pt

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 Ilhavo 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 \pm 0.01 μ g/L), long-term exposure may still pose risks to ecosystem functioning, ultimately affecting the quality of life of aquatic organisms.

Acknowledgements: This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020).

[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.



20 - 21 October, 2025 - Aveiro

P2

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

I.Rosco^{1*}, A. Almeida², A.R. Zizzamia¹, <u>F. Lelario</u>¹, V. Calisto²

¹University of Basilicata, 85100 Potenza, Italy

²University of Aveiro, 3810-193 Aveiro, Portugal

*incoronata.rosco@studenti.unibas.it

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 \pm 0.7% in ultrapure water and of 42 \pm 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.

Acknowledgements: This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020).

- [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.



20 - 21 October, 2025 - Aveiro

Р3

Evaluation of electrochemical degradation using a platinum anode for venlafaxine removal

Angelica R. Zizzamia¹, Veronica Pasquariello¹, <u>Filomena Lelario¹</u>*, Incoronata Rosco¹, Carmen Tesoro¹, Rosanna Ciriello¹

¹Department of Basic and Applied Sciences, University of Basilicata, 85100 Potenza, Italy *filomena.lelario@unibas.it

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 Na₂SO₄ electrolyte at pH 9 under galvanostatic conditions, applying a constant current density of 25 mA/cm². 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.; Mackul'ak, T.; Vojs Stařiová, 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.



20 - 21 October, 2025 - Aveiro

P4

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

Joanna Dołżonek1*, Piotr Stepnowski1

¹Department of Environmental Analysis, Faculty of Chemistry, University of Gdańsk, Wita Stwosza 63, 80-308 Gdańsk, Poland

*joanna.dolzonek@ug.edu.pl

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 CaCl₂), due to competition between Ca²⁺ 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.



20 - 21 October, 2025 - Aveiro

P5

MINIATURIZATION OF ECOTOXICOLOGICAL TESTS AND THEIR APPLICATION TO ASSESS THE TOXICITY OF \(\mathbb{G} \)-BLOCKERS TOWARDS CYANOBACTERIUM MICROCYSTIS AERUGINOSA

Maja Grabowska, Magda Caban*

University of Gdansk, Faculty of Chemistry, Department of Environmental Analysis, u. Wita Stwosza 63, 80-308 Gdańsk, Poland
*magda.caban@ug.edu.pl

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

Acknowledgements: Financial support was provided by the National Science Center (Poland) under grants UMO-2019/35/B/NZ9/00253.



20 - 21 October, 2025 - Aveiro

P6

TiO₂ photocatalyst supported on superparamagnetic silica aerogel for sunlight-activated removal of pharmaceuticals from wastewaters

<u>Fernanda Rodrigues</u>^{1,2,3*}, Maria Inês Roque², Cláudio M. R. de Almeida², Maria João Feio¹, Nuno E. C. Simões³, Luisa Durães²

¹University of Coimbra, MARE/ARNET, DCV/FCTUC, Largo Marquês de Pombal, 3004-517 Coimbra, Portugal.

²University of Coimbra, CERES, DEQ/FCTUC, Rua Sílvio Lima, 3030-790 Coimbra, Portugal.

³University of Coimbra, INESC Coimbra, DEC/FCTUC, Rua Luis Reis Santos, 3030-788 Coimbra, Portugal.

*fernanda.rodrigues@student.uc.pt

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 (SiO₂), 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 (TiO₂), 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 TiO₂ 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/m² (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.

Acknowledgements: This work was supported by the Foundation for Science and Technology, I. P. (FCT) and the European Social Fund [grant numbers 2022.14367.BD (DOI 10.54499/2022.14367.BD); 2024.03908.BDANA]. Work developed in CERES, under the strategic projects with DOIs 10.54499/UIDB/00102/2020 and 10.54499/UIDP/00102/2020, was funded by FCT and the European Regional Development Fund (ERDF), through COMPETE 2020.

- [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.



20 - 21 October, 2025 - Aveiro

P7

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

Anna Białk-Bielińska^{1*}, Joanna Dołżonek¹, Ewa Mulkiewicz¹, Jolanta Kumirska¹, Piotr Stepnowski¹

¹Department of Environmental Analysis, Faculty of Chemistry, University of Gdańsk, ul. Wita Stwosza 63, 80-308 Gdańsk, Poland

*anna.bialk-bielinska@ug.edu.pl

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.



20 - 21 October, 2025 - Aveiro

P8

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

Ensar Piskin^{1,2}, Ahmet Cetinkaya^{3,4}, Aytekin Uzunoglu⁵, Sibel A. Ozkan¹

¹Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

²Ankara University, Graduate School of Health Sciences, Ankara, Türkiye

³University of Health Sciences, Gülhane Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

⁴Hacettepe University Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

⁵Istanbul Technical University, Faculty of Chemical and Metallurgical Engineering, Department of

Metallurgical and Materials Engineering, İstanbul, Türkiye

*ensarpskn@qmail.com

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.



20 - 21 October, 2025 - Aveiro

P9

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

Beyza Unal^{1,2}, Fatma Budak¹, Ahmet Cetinkaya^{3,4}, Aytekin Uzunoglu⁵, Esen Bellur Atici^{6,7}, Sibel A. Ozkan¹

¹Ankara University, Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

²Ankara University, Graduate School of Health Sciences, Ankara, Türkiye

³University of Health Sciences, Gülhane Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

⁴Hacettepe University Faculty of Pharmacy, Department of Analytical Chemistry, Ankara, Türkiye

⁵Istanbul Technical University, Faculty of Chemical and Metallurgical Engineering, Department of

Metallurgical and Materials Engineering, İstanbul, Türkiye

⁶DEVA Holding A.S., R&D Center, Tekirdağ, Türkiye

⁷Gebze Technical University, Department of Chemistry, Kocaeli, Türkiye

*beyzaunal28@gmail.com

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.



20 - 21 October, 2025 - Aveiro

P10

Development of Copper Nanomaterials as Nanozymes for Advanced Water Treatment

Ana Rita Loureiro^{1*}, Vânia Calisto², Goreti Pereira², Ângela Almeida²

¹Department of Chemistry, University of Aveiro, Portugal

²Department of Chemistry & CESAM, University of Aveiro, Portugal

*aritaloureiro@ua.pt

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 \pm 4 nm, whereas Cu_{2-x}Se-MS are more elongated particles with irregularities on their surface, with average widths of 102 \pm 14 nm and lengths of 346 \pm 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.

Acknowledgements: This work was developed within the project SYNERGY (2022.02028.PTDC), supported by national funds (OE), through FCT/MCTES. This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020).

- [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.



20 - 21 October, 2025 - Aveiro

P11

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

Almeida, Â.^{1*}, Sousa, É. M. L.¹, Canha, T.², Freitas, R.³, Calisto, V.¹

¹Department of Chemistry and CESAM, University of Aveiro, 3810-193, Aveiro, Portugal

²Department of Physics, University of Aveiro, 3810-193, Aveiro, Portugal

³Department of Biology and CESAM, University of Aveiro, 3810-193, Aveiro, Portugal

*aaalmeida@ua.pt

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.

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).



20 - 21 October, 2025 - Aveiro

P12

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

Rita Gouveia^{1*}, Ângela Almeida², Érika M.L. Sousa², Francisco Freitas³, Vânia Calisto²

¹Department of Chemistry, University of Aveiro, Aveiro, Portugal ²Department of Chemistry and CESAM, University of Aveiro, Aveiro, Portugal ³Department of Chemistry and CICECO, University of Aveiro, Aveiro, Portugal * ritacggouveia@ua.pt

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.

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] 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



20 - 21 October, 2025 - Aveiro

P13

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

Maria Fernanda Nogueira^{1*}; Paula Paíga¹; Cristina Soares¹; Manuela Correia¹; Cristina Delerue-Matos¹

¹REQUIMTE/LAQV, Instituto Superior de Engenharia do Porto, Instituto Politécnico do Porto, Rua Dr.

António Bernardino de Almeida, 431, 4249-015 Porto, Portugal

*mffna@isep.ipp.pt

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 μ g/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.

Acknowledgements: Maria Fernanda Nogueira gratefully acknowledges FCT/MECI for the PhD fellowship 2024.15665.PRT. This work received financial support from national funds (FCT/MECI) through the project UID/50006 - Laboratório Associado para a Química Verde - Tecnologias e Processos Limpos.

- [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.



20 - 21 October, 2025 - Aveiro

P14

Application of magnetic TiO₂/Carbon Quantum Dots for efficient removal of antibiotics from water

V. Silva1*, M. Otero2, V. Calisto1, D.L.D. Lima1,3

¹CESAM & Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro, Portugal ²Departmento de Química y Física Aplicadas, Universidad de León, Campus de Vegazana, 24071 León, España

³H&TRC - Health & Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, Rua 5 de Outubro – S. Martinho do Bispo, 3046-854 Coimbra, Portugal *e-mail address: valentinagsilva@ua.pt

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 TiO2, Carbon Quantum Dots (CQD) and magnetic nanoparticles was produced using a co-precipitation methodology. The produced magnetic TiO₂/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 TiO₂/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 $47 \pm 4\%$ and $44 \pm 7\%$ of AMX and TMP, respectively, in 0.4 h irradiation, and $40 \pm$ 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 TiO₂/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 TiO₂/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.

Acknowledgements: Valentina Silva thanks FCT support for the individual PhD grant (2022.10472.BD, https://doi.org/10.54499/2022.10472.BD). Diana L.D. Lima thanks support by Fundação para a Ciência e a **SOLCAT** (2023.12723.PEX, Tecnologia (FCT) the research project to https://doi.org/10.54499/2023.12723.PEX). This work is funded by national funds through FCT - Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020) of UID Centro de Estudos do Ambiente e Mar and UIDP/05608/2020 (https://doi.org/10.54499/UIDP/05608/2020) UIDB/05608/2020 (https://doi.org/10.54499/UIDB/05608/2020) of H&TRC.



20 - 21 October, 2025 - Aveiro

P15

Adsorption and Biocatalysis Synergy for Water Treatment: a laccasebiochar composite for diclofenac removal from water

Hugo F. Rocha^{1*}, Ângela Almeida¹, Goreti Pereira¹, M. Rosário Domingues¹, Diana L. D. Lima², Vânia Calisto²

¹Department of Chemistry and CESAM, University of Aveiro, 3810-193, Aveiro, Portugal

²H&TRC – Health and Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, Rua 5 de Outubro, S. Martinho do Bispo, 3054-854, Coimbra, Portugal.

*Email: hugofmr@ua.pt

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 °C, N2 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 °C, 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(-)MS² 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 Lacfunctionalized 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.

Acknowledgements: This work was developed within the project SYNERGY (2022.02028.PTDC), supported by national funds (OE), through FCT/MCTES. This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020). Diana Lima also acknowledges financial support to H&TRC by FCT/MCTES (UIDP/05608/2020 (https://doi.org/10.54499/UIDP/05608/2020) and UIDB/05608/2020 (https://doi.org/10.54499/UIDB/05608/2020)).



20 - 21 October, 2025 - Aveiro

P16

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

Zoltán Konthur¹, Maximilian Lehnert¹, Shireen Ewald¹, Caitlin Hartlage¹, Doğa İkizoğulları¹,

Thomas Exner², Marcus Lukas², Ulrike Braun², Rudolf J. Schneider^{1*}

¹BAM Federal Institute for Materials Research and Testing, 12205 Berlin, Germany

²UBA Federal Environment Agency, 12307 Berlin, Germany

*rudolf.schneider@bam.de

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.

Acknowledgements: The data was obtained through the EU-funded project ESI-CorA (Emergency Support Instrument – Detection of SARS-CoV-2 in Wastewater) and the German governmental initiative AMELAG (Wastewater Monitoring for Epidemiological Situation Assessment [6]).

- [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



20 - 21 October, 2025 - Aveiro

P17

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

A.R. Zizzamia^{1*}, Â. Almeida², M.V. Gil³, F. Lelario¹, V. Calisto²

¹University of Basilicata, 85100 Potenza, Italy

²Department of Chemistry & CESAM, University of Aveiro, 3810-193 Aveiro, Portugal

³Instituto de Ciencia y Tecnología del Carbono, INCAR (CSIC), Oviedo, Spain

*angelicarebecca.zizzamia@unibas.it

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 $90.3\% \pm 0.08\%$ for SILD and $94.6\% \pm 2.14\%$ 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.

Acknowledgements: This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P. under the project/grant UID/50006 + LA/P/0094/2020. The authors also thank Faustino Microcervejeira, Lda. (Aveiro, Portugal) and its head brewer for kindly providing the brewing residues used in this work.

- [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.



20 - 21 October, 2025 - Aveiro

P18

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

<u>Grazia Accoto¹</u>, Dominga Bochicchio^{1*}, Annunziata Marraudino¹, Katarzyna Pilat¹, Achille Palma¹

*ARPA Basilicata, Italy
*dominga.bochicchio@arpab.it

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.



20 - 21 October, 2025 - Aveiro

P19

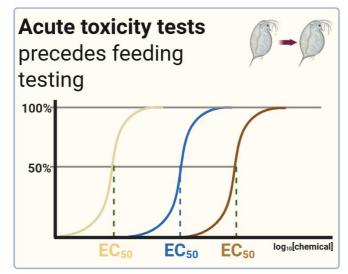
Feeding as a phenotypic endpoint to identify the impact of pharmaceuticals in environmentally low concentrations

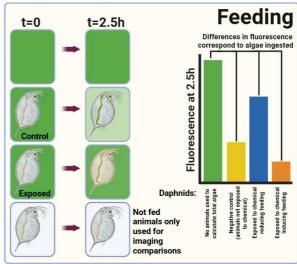
Emma Rowan^{1*}, Anne Leung¹, Flavia Melati Chiappara¹, Izabela Malgorzata Antepowicz¹, Maria Eleni Tsioli¹, Konstantinos Grintzalis¹

¹School of Biotechnology, Dublin City University, Ireland *emma.rowan4@mail.dcu.ie

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.



20 - 21 October, 2025 - Aveiro

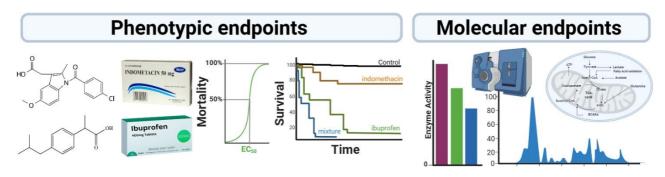
P20

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

<u>Flavia Melati Chiappara*</u>, Izabela Malgorzata Antepowicz, Maria Eleni Tsioli, Anne Leung, Emma Rowan, Konstantinos Grintzalis

¹School of Biotechnology, Dublin City University, Ireland *flavia.melatichiappara2@mail.dcu.ie

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.





20 - 21 October, 2025 - Aveiro

P21

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

<u>Guilherme F. Pinto</u>^{1,2}, Patrick Krebs², Claudete F. Pereira³, Giovannia A. L. Pereira³, Vânia Calisto⁴, Boris Mizaikoff², Goreti Pereira⁴

¹Department of Chemistry, University of Aveiro, Aveiro, Portugal.

²Institute of Analytical and Bioanalytical Chemistry, Ulm University, Ulm, Germany.

³Department of Fundamental Chemistry, Federal University of Pernambuco, Recife, Brazil.

⁴Department of Chemistry & CESAM, University of Aveiro, Aveiro, Portugal.

*guilhermepinto@ua.pt

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 $\mu g/mL$ range. This work demonstrates the potential of Ag₂Se 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.

Acknowledgements: The authors acknowledge financial support from FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020, the project NanoSEIRA (COMPETE2030-FEDER-00866600), as well as the Erasmus+ program and the DAAD (German Academic Exchange Service) for enabling the research exchange.



20 - 21 October, 2025 - Aveiro

P22

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

Dinis Costa¹, <u>Diana Bordalo</u>², Marta Cunha², Amadeu MVM Soares², Susana Carvalho³, Rosa Freitas^{2*}

¹Department of Biology, University of Aveiro 3810-193, Aveiro, Portugal

²Department of Biology & CESAM, University of Aveiro 3810-193, Aveiro, Portugal

³Red Sea Research Center, King Abdullah University of Science and Technology, Thuwal 23955, Kingdom of Saudi Arabia

*rosafreitas@ua.pt

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 speciesand 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.

Acknowledgements: Diana Bordalo and Marta Cunha benefited from PhD grants (2023.01230.BD and 2024.01100.BD, respectively) given by the National Funds through the Portuguese Science Foundation (Fundação para a Ciência e a Tecnologia, FCT). This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020



20 - 21 October, 2025 - Aveiro

P23

Pistia stratiotes L. (Araceae) exposed to amoxicillin: implications for ecotoxicological risk assessment in aquatic systems

<u>Lucélia Hoehne^{1,2*}</u>, Elziane Pereira Ferro¹, Joana Elisa Willrich¹, Gabriela Thaís Lehnen Mendes², Ani Caroline Weber¹, Jéssica Samara Herek dos Santos¹, Ana Giacomin¹, Ikram Bashir¹, Elisete Maria de Freitas¹, Ana Paula Mora Tavares³, Ana Maria Ferreira Takahashi³

¹ Valley of Taquari University - Univates, Graduate Program in Biotechnology, Avelino Tallini, 171, room 309 buid 8, Lajeado, RS, Brazil, Zip code: 95914-014

² Valley of Taquari University - Univates, Graduate Program in Environmental and Development, Avelino Tallini, 171, room 309 build 8, Lajeado, RS, Brazil, Zip code: 95914-014 ³CICECO, Department of Chemistry, University of Aveiro, 3810-193, Aveiro, Portugal. *luceliah@univates.br

The continuous release of pharmaceuticals into aquatic environments, particularly antibiotics such as amoxicillin, raises concerns regarding their potential ecotoxicological effects on non-target aquatic organisms. These contaminants reach water bodies mainly through domestic sewage, effluents from pharmaceutical industries, and inadequate disposal of unused medications. Due to their persistent nature and biological activity, antibiotics may alter the ecological balance of aquatic ecosystems, even at low concentrations. In this context, aquatic macrophytes have gained attention as effective bioindicators of water quality [1]. Among them, Pistia stratiotes L. (Araceae) stands out due to its wide distribution, rapid growth, and sensitivity to environmental changes. As primary producers, macrophytes play a crucial role in aquatic ecosystems, and disruptions to their physiological processes—such as pigment synthesis—can reflect broader ecological disturbances. Therefore, investigating photosynthetic pigment alterations in P. stratiotes under antibiotic stress provides valuable insights into sublethal toxic effects. Pigment profiling, including chlorophylls and carotenoids, is a non-destructive and sensitive approach that can reveal early signs of stress before visible symptoms or growth impairments occur [2]. This study aimed to evaluate the impact of amoxicillin on P. stratiotes, focusing on alterations in photosynthetic pigments as potential biomarkers of stress. P. auriculata specimens were exposed to 20 mL of amoxicillin solution at concentrations of 5, 50 and 100 mg/L in Petri dishes, each containing five plants, in triplicate, for 24 hours. After the exposure period, the levels of chlorophyll a, chlorophyll b, and carotenoids were quantified and compared to a control group (no pharmaceutical exposure). The results showed a marked reduction in chlorophyll a content (from 322 to 200 µg/g), suggesting impaired photosynthetic efficiency. Conversely, chlorophyll b and carotenoids increased (from 99 to 115 µg/g and from 21 to 49 µg/g, respectively), indicating a possible compensatory mechanism to maintain light harvesting and mitigate oxidative stress. These findings highlight the sensitivity of P. stratiotes to antibiotic exposure and support the use of pigment profiling as an effective tool in ecotoxicological risk assessment. Further investigations involving oxidative stress markers and growth parameters are recommended to better understand the sublethal effects of pharmaceutical pollutants in freshwater ecosystems.

Acknowledgements:

Brazilian Coordination for the Improvement of Higher Education Personnel (CAPES), National Council for Scientific and Technological Development (CNPq) CICECO – Aveiro Institute of Materials, financed by national funds through FCT/MCTES (PIDDAC).

- [1] Okoye C. O. et al., Environmental Toxicology and Pharmacology, v. 96, 2022, 103995.
- [2] Samal, K. and Dash, R. R. Science of the Total Environment, v. 926, p. 171981, 2024.



20 - 21 October, 2025 - Aveiro

P24

Green synthesis of silver and copper QDs as promising radiopharmaceuticals

Zélia Barbosa^{1,*}, Antero Abrunhosa², Goreti Pereira³

¹Polytechnic University of Coimbra, Coimbra Health School, Rua 5 de Outubro, S. Martinho do Bispo, 3046-854 Coimbra, Portugal. ²Institute for Nuclear Sciences Applied to Health (ICNAS), University of Coimbra, Portugal. ³Department of Chemistry & CESAM, University of Aveiro, Portugal. *zeliabarbosa@estesc.ipc.pt

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 Ag₂Se 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] Krecisz, P. et al. Journal of Medicinal Chemistry, 2025, 68, 2356



20 - 21 October, 2025 - Aveiro

P25

Synthesis of nadifloxacin derivatives for further ecotoxicological studies

Igor E. Oliveira¹, Ana R. L. Ribeiro^{2,3}, Maria E. Tiritan^{1,4,5*}

¹ Laboratory of Organic and Pharmaceutical Chemistry, Department of Chemical Sciences, Faculty of Pharmacy, University of Porto, 4050-313, Porto, Portugal

 ² LSRE-LCM - Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal
 ³ ALiCE - Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

⁴ CIIMAR/CIMAR LA, Interdisciplinary Centre of Marine and Environmental Research, University of Porto, Terminal de Cruzeiros do Porto de Leixões, 4450-208 Matosinhos, Portugal
 ⁴ UCIBIO-Applied Molecular Biosciences Unit, Translational Toxicology Research Laboratory, University Institute of Health Sciences (1H-TOXRUN, IUCS-CESPU), Gandra, Portugal
 *e-mail: beth@ff.up.pt

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.

Acknowledgements: This work is financially supported by national funds through the FCT/MCTES (PIDDAC), under the projects: 2022.02842.PTDC - STAR - STereoselective environmental processes in Antibiotics: role for Resistance, with DOI 10.54499/2022.02842.PTDC (https://doi.org/10.54499/2022.02842.PTDC), 2022.08738.PTDC - DRopH2O - Drinking water quality: early warning and removal of microcontaminants by 10.54499/2022.08738.PTDC carbon-based materials with DOI (https://doi.org/10.54499/2022.08738.PTDC); and also UIDB/04423/2020 (https://doi.org/10.54499/UIDB/04423/2020), UIDP/04423/2020 (https://doi.org/10.54499/UIDP/04423/2020), LA/P/0101/2020 (https://doi.org/10.54499/LA/P/0101/2020) (Group of Marine Natural Products and Medicinal Chemistry); LSRE-LCM, UID/50020/2025, and ALiCE, LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020).

- [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.



20 - 21 October, 2025 - Aveiro

P26

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

<u>Fabiana Y. M. Vieira</u>^{1,2}, Diana Carneiro¹, Maria D. Pavlaki¹, Roberto Martins¹, João Tedim² and Susana Loureiro¹

¹CESAM – Centre for Environmental and Marine Studies and Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal.

²CICECO - Centre for Research in Ceramics and Composite Materials and DEMaC – Department of Materials and Ceramics Engineering, University of Aveiro, 3810-193 Aveiro, Portugal.

*fyvieira@ua.pt

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, LC₅₀ 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.

Acknowledgements: This work was funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P. to: CESAM - Centro de Estudos do Ambiente e Mar under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020); CICECO-Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020); F. Y. M. Vieira (PhD grant 2020.05408.BD; DOI 10.54499/2020.05408.BD); D. Carneiro (PhD grant 2021.06691.BD, DOI 10.54499/2021.06691); M. Pavlaki (grant ref.: 2023.06417.CEECIND/CP2840/CT0014; DOI: 10.54499/2023.06417.CEECIND/CP2840/CT0014) and R. Martins (grant ref.: 2021.00386.CEECIND; DOI: 10.54499/2021.00386.CEECIND/CP1659/CT0011).



20 - 21 October, 2025 - Aveiro

P27

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

Leonor R. Barroca^{1,2+}, Joaquín A. Marrero^{1,2}, Ana M. Gorito^{1,2}, Adrián M.T. Silva^{1,2}, Ana Rita L. Ribeiro^{1,2*}

¹ LSRE-LCM – Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

*Presenting author: lcbarroca@fe.up.pt *Corresponding author: ritalado@fe.up.pt

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 μ g/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.

Acknowledgements: This work was supported by national funds through the FCT/MCTES (PIDDAC) under Project STAR, 2022.02842.PTDC (DOI: 10.54499/2022.02842.PTDC); by UID/50020/2025 of LSRE-LCM - Laboratory of Separation and Reaction Engineering – Laboratory of Catalysis and Materials - funded by FCT, I.P./MCTES through national funds; and ALiCE - LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020). This work was also supported by the European Commission through the European Research Council Executive Agency under the Grant Agreement 101039270 – Project ERA-ARE – (ERC-2021-STG). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or ERC Executive Agency. Neither the European Union nor the granting authority can be held responsible for them. ARLR acknowledges the FCT funding received under the 5th Scientific Employment Stimulus-Individual Call (2022.00184.CEECIND, with DOI: 10.54499/2022.00184.CEECIND/CP1733/CT0001).

- [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.

² ALiCE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.



20 - 21 October, 2025 - Aveiro

P28

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

<u>Beatriz Suordem</u>^{1,2,3,4*}, Leonor R. Barroca^{2,3}, Joaquín A. Marrero^{2,3}, Ana M. Gorito^{2,3}, Marta O. Barbosa^{2,3}, Maria Elizabeth Tiritan^{4,5,6,7}, Cláudia Ribeiro^{4,5}, and Ana Rita L. Ribeiro^{2,3}

¹Department of Public Health and Forensic Sciences, and Medical Education, Faculty of Medicine, University of Porto, Alameda Prof. Hernâni Monteiro, 4200-319 Porto, Portugal;

²LSRE-LCM – Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;
³ALICE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal;

⁴Associate Laboratory i4HB – Institute for Health and Bioeconomy, University Institute of Health Sciences - CESPU, 4585-116 Gandra, Portugal;

 ⁵UCIBIO – Applied Molecular Biosciences Unit, Translational Toxicology Research Laboratory University Institute of Health Sciences (1H-TOXRUN, IUCS-CESPU), 4585-116 Gandra, Portugal;
 ⁶Laboratory of Organic and Pharmaceutical Chemistry, Department of Chemical Sciences, Faculty of Pharmacy, University of Porto, Rua de Jorge Viterbo Ferreira, 4050-313 Porto, Portugal;
 ⁷CIIMAR/CIMAR LA, Interdisciplinary Centre of Marine and Environmental Research, University of Porto, Terminal de Cruzeiros do Porto de Leixões, 4450-208 Matosinhos, Portugal
 * up202203432@edu.med.up.pt

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.

Acknowledgements:

This work was supported by national funds through the FCT/MCTES (PIDDAC) under Project STAR, 2022.02842.PTDC (DOI: 10.54499/2022.02842.PTDC); by LSRE-LCM, UID/50020/2025; and ALiCE, LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020). Additionally, this work was also partially supported by FCT/MCTES (PIDDAC) via institutional funding to the associate laboratory UCIBIO (DOI: 10.54499/LA/P/0140/2020) - Associate Laboratory i4HB and through the annual funding of 1H-TOXRUN of the University Institute of Health Sciences (IUCS-CESPU) and CIIMAR within the scope of the Strategic Funding UIDB/04423/2020 (https://doi.org/10.54499/UIDB/04423/2020), UIDP/04423/2020 (https://doi.org/10.54499/UIDP/04423/2020), and LA/P/0101/2020 (https://doi.org/10.54499/LA/P/0101/2020). ARLR and MOB acknowledge the support from FCT funding under the Scientific Employment Stimulus—Ind. Call (DOI: 10.54499/2022.00184.CEECIND/CP1733/CT0001 and 10.54499/2023.07147.CEECIND/CP2834/CT0003), respectively.

- [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



20 - 21 October, 2025 - Aveiro

P29

Selection of ofloxacin-degrading microorganisms from activated sludge microbiota

<u>Joaquín A. Marrero^{1,2*}</u>, Ana S. Oliveira^{1,2}, Ana M. Gorito^{1,2}, Adrián M.T. Silva^{1,2}, Olga C. Nunes^{2,3}, Ana Rita L. Ribeiro^{1,2}

 ¹ LSRE-LCM – Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.
 ² ALiCE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.

³ LEPABE – Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal. *up201604408@fe.up.pt

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.

Acknowledgements:

This work was supported by the European Commission through the European Research Council Executive Agency under the project 101039270 — ERA-ARE — ERC-2021-STG, funded by the European Union. *Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or ERC Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.* This research was also supported by Fundação para a Ciência e a Tecnologia, I.P. /MCTES through national funds: LSRE-LCM, UID/50020/2025; ALiCE - LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020); and project 2022.02842.PTDC — STAR - STereoselective environmental processes in Antibiotics: role for Resistance, with DOI 10.54499/2022.02842.PTDC (https://doi.org/10.54499/2022.02842.PTDC). ARLR acknowledges the FCT funding received under the 5th Scientific Employment Stimulus-Individual Call (2022.00184.CEECIND, with DOI: 10.54499/2022.00184.CEECIND/CP1733/CT0001).

- [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/



20 - 21 October, 2025 - Aveiro

P30

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

Diana Carneiro¹, Daniel Bruno¹, Madalena Vieira¹, Inês Pereira², Érika Sousa³, Vânia Calisto³, Marta Martins², Roberto Martins¹, Susana Loureiro¹, Maria D. Pavlaki¹

¹CESAM-Centre for Environmental and Marine Studies & Department of Biology, University of Aveiro, 3810-193 Aveiro, Portugal

²Marine and Environmental Sciences Centre (MARE), Department of Environmental Sciences and Engineering, NOVA School of Science and Technology, NOVA University Lisbon (FCT NOVA), 2829-516 Caparica, Portugal

³CESAM-Centre for Environmental and Marine Studies & Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

*maria.pavlaki@ua.pt

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 μ g/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 μ g/L. Regarding gene expression, epirubicin exposure (500 μ g/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.

Acknowledgements: This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020). FCT also financed the doctoral grant to D. Carneiro (2021.06691.BD), and the researcher grants to R. Martins (2021.00386.CEECIND; DOI: 10.54499/2021.00386.CEECIND/CP1659/CT0011) and M. Pavlaki (2023.06417.CEECIND/CP2840/CT0014; DOI: 10.54499/2023.06417.CEECIND/CP2840/CT0014). The present work was supported by the project VitroTox (PTDC/CTA-AMB/0126/2020, DOI: 10.54499/PTDC/CTA-AMB/0126/2020)), financed by national funds (OE), through FCT.



20 - 21 October, 2025 - Aveiro

P31

Selective antibacterial effects of fluoroquinolones on wastewater bacteria

Alexandre van Heerden^{1,2*}, Ana S. Oliveira^{1,2}, Ana M. Gorito^{1,2}, Olga C. Nunes^{2,3}, Ana Rita L. Ribeiro^{1,2}

¹LSRE-LCM – Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal. ²ALiCE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.

³LEPABE – Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal. * aheerden@fe.up.pt

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 broadspectrum 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 taxonspecific 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.

Acknowledgments: This work was supported by Project ERA-ARE (ERC-2021-STG) funded by the European Commission under the Grant Agreement 101039270 of European Research Council Executive Agency. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or ERC Executive Agency. Neither the European Union nor the granting authority can be held responsible for them. This work was also supported by: Project STAR, 2022.02842.PTDC 10.54499/2022.02842.PTDC) through the FCT/MCTES (PIDDAC); LSRE-LCM, UID/50020/2025; and ALiCE, LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020). ARLR acknowledges the

FCT funding 2022.00184.CEECIND, with DOI: 10.54499/2022.00184.CEECIND/CP1733/CT0001).

- [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.



20 - 21 October, 2025 - Aveiro

P32

Incorporation of TiO₂/CQDs into polymeric fibers for the photodegradation of amoxicillin in water

<u>Beatriz Valadares</u>^{1,2*}, Valentina Silva³, Rosa Baptista⁴, Bernardo Almeida⁴, Diana Lima³,⁵, Vânia Calisto³, Goreti Pereira³

¹Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal. ²Polytechnic Institute of Coimbra, Coimbra Health School, Rua 5 de Outubro – S. Martinho do Bispo, Apartado 7006, 3046-854 Coimbra, Portugal

³Department of Chemistry and CESAM, University of Aveiro, 3810-193 Aveiro, Portugal, ⁴Centre of Physics of Minho and Porto Universities (CF-UM-UP), Laboratory for materials and Emergent Technologies (LAPMET), University of Minho, 4710-057 Braga, Portugal.

⁵4H&TRC - Health & Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, 3045-043, Coimbra, Portugal

* beatriz.valadares@ua.pt

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/TiO₂/CQD fibers can be a promising and sustainable approach to remove antibiotics from water environments.

Acknowledgements: This work is funded by national funds through FCT – Fundação para a Ciência e a Tecnologia I.P., under the project/grant UID/50006 + LA/P/0094/2020 (doi.org/10.54499/LA/P/0094/2020). Valentina Silva thanks FCT support for the individual PhD grant (2022.10472.BD, https://doi.org/10.54499/2022.10472.BD). This research was also funded by FCT through FEDER (European Fund for Regional Development)-COMPETE-QREN-EU (ref. UID/FIS/04650/2013 and UID/FIS/04650/2019). Diana L.D. Lima thanks support by Fundação para a Ciência e a Tecnologia (FCT) to the SOLCAT research project (2023.12723.PEX, https://doi.org/10.54499/2023.12723.PEX).



20 - 21 October, 2025 - Aveiro

P33

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

<u>Joana F. M. Sousa^{1,*}</u>, Paulo E. Abreu¹, Artur J. M. Valente¹, Jorge M. C. Marques¹

¹University of Coimbra, CQC-IMS, Department of Chemistry, Rua Larga 3004-535, Coimbra, Portugal.

*UC2011141774@student.uc.pt

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.

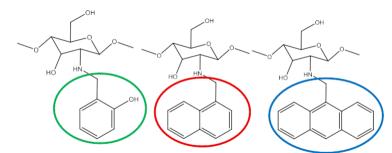


Figure 1: Structure of chitosan functionalized by salicylaldehyde (RCS) green circle in the left, naphthaldehyde (RCN) red circle in middle and 9-anthracenecarboxaldehyde (RCA) blue circle in the right.

Acknowledgements: We thank Fundação para a Ciência e Tecnologia (FCT), Portugal for the Ph. D Grant UI/BD/150803/2020 with DOI 10.54499/UI/BD/150803/2020 (https://doi.org/ 10.54499/UI/BD/150803/2020) and the Coimbra Chemistry Center (CQC), supported by the FCT through Projects UIDB/00313/2025 and UIDP/00313/2025, for supporting this work. The authors are also grateful for the provision of computational time in the supercomputer resources hosted at Laboratório de Computação Avançada (2023.10661.CPCA.A1, DOI 10.54499/2023.10661.CPCA.A1) which was financed by FCT.

- [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.



20 - 21 October, 2025 - Aveiro

P34

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

Inês M. Quintela^{1*}, Ana M. Gorito¹, Marta O. Barbosa¹, Ana R.L. Ribeiro¹, Adrián M.T. Silva¹

¹LSRE-LCM, ALiCE, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.

*up202006309@up.pt

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 μ g 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.

Acknowledgements:

This work was supported by national funds through FCT/MCTES (PIDDAC), under the projects DRopH $_2$ O, 2022.08738.PTDC (DOI: 10.54499/2022.08738.PTDC, https://doi.org/10.54499/2022.08738.PTDC), and STAR, 2022.02842.PTDC (DOI: 10.54499/2022.02842.PTDC, https://doi.org/10.54499/2022.02842.PTDC). This research was also supported by Fundação para a Ciência e a Tecnologia, I.P./MCTES through national funds: LSRE-LCM, UID/50020; and ALiCE, LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020). ARLR and MOB acknowledge the support from FCT funding under the Scientific Employment Stimulus–Ind. Call (DOI: 10.54499/2022.00184.CEECIND/CP1733/CT0001 and 10.54499/2023.07147.CEECIND/CP2834/CT0003), respectively.

- [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.



20 - 21 October, 2025 - Aveiro

P35

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

Paulo M.S. Sousa^{1,2,*}, Manuel Simões^{1,2}, Cátia A. Sousa^{1,2,3,4}

¹LEPABE - Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

²ALiCE - Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal

³ISEP/P.PORTO, School of Engineering, Polytechnic of Porto, Rua Dr. António Bernardino de Almeida, 431, 4249-015, Porto, Portugal

⁴CIETI, ISEP/P.PORTO, School of Engineering, Polytechnic of Porto, Rua Dr. António Bernardino de Almeida, 431, 4249-015, Porto, Portugal

* up201206729@edu.fe.up.pt

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 microalgaebased 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.

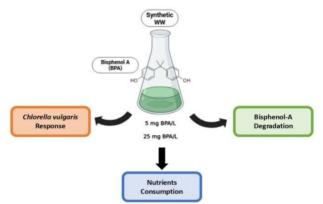


Figure 1: The potential of Chlorella vulgaris to bioremediate a wastewater contaminated with Bisphenol-A, at relevant environmental concentrations.

Acknowledgements: This work was supported by national funds through FCT/MCTES (PIDDAC): LEPABE, UIDB/00511/2020 (DOI: 10.54499/UIDB/00511/2020), UIDP/00511/2020 (DOI:10.54499/UIDP/00511/2020), and ALiCE, LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020); the grant attributed by Portuguese Foundation for Science and Technology, I.P. – FCT – to Paulo Sousa by project reference 2022.14159.BD and DOI:10.54499/2022.14159.BD.

- [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



20 - 21 October, 2025 - Aveiro

P36

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

Gitte Van de Weyer¹, Valentina Silva², Ana Paula Fonseca^{3,4}, Diana L.D. Lima^{3,4}, Carla Patrícia Silva^{3,4,*}

¹Thomas More University of Applied Sciences, Campus Thomas More Geel, 2440 Geel, Belgium

²Department of Chemistry and CESAM, University of Aveiro, 3810-193 Aveiro, Portugal

³Polytechnic University of Coimbra, 3045-093 Coimbra, Portugal

⁴H&TRC - Health & Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra, 3045-043, Coimbra, Portugal

*carla.silva@estesc.ipc.pt

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 (TiO₂) 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 ultraviolet detection (HPLC-UV) was used to quantify antibiotic concentrations in aqueous solution before and after the photocatalyst application.

Results showed that magnetic CQDs-TiO₂ composites had compound-specific behavior. For TMP, magnetic CQDs-TiO₂ significantly enhanced degradation efficiency, as indicated by lower antibiotic concentration in aqueous solution, compared with the results obtained using magnetic TiO₂ composites (without CQDs incorporation). In contrast, magnetic CQDs-TiO₂ did not improve SMX degradation and in some cases the incorporation of CQDs in the magnetic TiO₂ 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.

Acknowledgements:

This work was financed by national funds through FCT – Foundation for Science and Technology, I.P., within the scope of the project 2023.12723.PEX. DOI: https://doi.org/10.54499/2023.12723.PEX.



20 - 21 October, 2025 - Aveiro

P37

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

Andreia Carvalho¹, Diana L.D. Lima^{1,2}, Carla Patrícia Silva^{1,2}, <u>Ana Paula Fonseca^{1,2,*}</u>

¹Polytechnic University of Coimbra, 3045-093 Coimbra, Portugal

²H&TRC - Health & Technology Research Center, Coimbra Health School, Polytechnic University of Coimbra.

3045-043, Coimbra, Portugal *paula fonseca@estesc.ipc.pt

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.

Acknowledgements: This work was financed by national funds through FCT – Foundation for Science and Technology, I.P., within the scope of the project 2023.12723.PEX. DOI: https://doi.org/10.54499/2023.12723.PEX.



20 - 21 October, 2025 - Aveiro

P38

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

Belén González 12, Judit Kalman 34, Iván Dorado 3, Yolanda Valcárcel 34

¹ Department of Analytical Chemistry, University of the Basque Country (UPV/EHU), Spain ² Research Centre for Experimental Marine Biology and Biotechnology, University of the Basque Country (PiE-UPV/EHU), Spain

³Research group on human and environmental risk (RISAMA) and Department of Medical Specialities and Public Health. Faculty of Health Sciences, Rey Juan Carlos University, Alcorcón (Madrid), Spain ⁴Department of Medical Specialities and Public Health. Faculty of Health Sciences, Rey Juan Carlos University.28922 Alcorcón (Madrid), Spain

*yolanda.valcarcel@urjc.es

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. A mong 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.

Acknowledgements: To the Own Program for the Promotion and Development of Research and Innovation of Rey Juan Carlos University (Bridge Projects), 2024. Also thank to Canal Isabel II and the Research Centre for Experimental Marine Biology and Biotechnology, University of the Basque Country (PiE-UPV/EHU), Spain.



20 - 21 October, 2025 - Aveiro

P39

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

Isabel Brás^{1,*}, Elisabete Silva ^{1,2}

¹Polytechnic University of Viseu – ESTGV, Campus Politécnico, Repeses, 3504-510, Viseu, Portugal, CISeD Research Centre, Polytechnic University of Viseu – ESTGV, Campus Politécnico, Repeses, 3504-510, Viseu, Portugal

²LEPABE-Laboratory for Process Engineering, Environment, Biotechnology and Energy, Faculty of Engineering, University of Porto (FEUP), R. Dr. Roberto Frias S/N, 4200-465 Porto, Portugal *ipbras@estgv.ipv.pt

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.

Acknowledgements: This work was financed by National Funds through FCT - Foundation for Science and Technology, I.P., under the project Ref.^a UIDB/05583/2020. We additionally thank the Digital Services Research Center (CISeD) and the Polytechnic Institute of Viseu for the support provided.

List of Participants

Name	Email	Institution
Abraham Esteve-Núñez	Abraham.esteve@uah.es	University of Alcalá
Achille Palma	achille.palma@arpab.it	ARPAB
Ahmet Cetinkaya	ahmet.cetinkya@yahoo.com	Ankara University
Alexandre Daniel Fernandes van Heerden	up202103731@up.pt	FEUP
Alyson Rogério Ribeiro	alysonrogerio@ufmg.br	Federal University of Minas Gerais
Ana Luísa Patrício Silva	ana.luisa.silva@ua.pt	Universidade de Aveiro
Ana Paula Gomes Fonseca	paula_fonseca@estesc.ipc.pt	ESTESC
Ana Rita Lado Teixeira Ribeiro	ritalado@fe.up.pt	FEUP
Ana Rita Moreira Loureiro	aritaloureiro@ua.pt	Universidade de Aveiro
Ana Sofia Teixeira Oliveira	atoliveira@fe.up.pt	FEUP
André Monteiro Pais Teixeira Pereira	andrepereira@ff.uc.pt	Universidade de Coimbra
Ângela Augusta Soares de Almeida	aaalmeida@ua.pt	Universidade de Aveiro
Angelica Rebecca Zizzamia	angelicarebecca.zizzamia@unibas.it	University of Basilicata
Anna Białk-Bielińska	anna.bialk-bielinska@ug.edu.pl	University of Gdańsk
Anne-Lise Bienvenu	anne-lise.bienvenu@chu-lyon.fr	Université Lyon
Beatriz Antunes Camarneiro	beatriz.antunes@ua.pt	Universidade de Aveiro
Beatriz Gonçalo Leal Suordem	up202203432@edu.med.up.pt	FEUP
Beatriz Nunes da Silva Valadares	beatriz.valadares@ua.pt	Instituto Politécnico de Coimbra
Beyza Unal	beyzaunal28@gmail.com	Ankara University
Carla Patrícia Gonçalves Silva	patricia.silva@ua.pt	ESTESC
Carolina Almeida Machado	carolina02@ua.pt	Universidade de Aveiro
Célia Valadas Frazão Duarte	cfduarte@hovione.com	Hovione
Chiara Ilgrande	cilgrande@aimplas.es	Aimplas
Cigdem Kalkan Aktan	cigdemkalkan@marmara.edu.tr	Marmara University
Damià Barceló	damiab@ual.es	University of Almeria
Daniel Ettlin	daniel.ettlin@thermounicam.pt	Unicam
Diana Aga	dianaaga@buffalo.edu	University at Buffalo
Diana Luísa Duarte de Lima	diana.lima@ua.pt	ESTESC
Diana Vanessa Martins Bordalo	dianabordalo@ua.pt	Universidade de Aveiro
Diogo Esteves Pereira	diogoepereira@ua.pt	Universidade de Aveiro
Dominga Bochicchio	dominga.bochicchio@arpab.it	ARPA Basilicata
Emma Rowan	emma.rowan4@mail.dcu.ie	Dublin City University
Ensar Piskin	ensarpskn@gmail.com	Ankara University
Érika Maria Leite de Sousa	erikamsousa@ua.pt	Universidade de Aveiro
Fabiana Yamasaki Martins Vieira	fyvieira@ua.pt	University of Aveiro
Farah Masoud Elbarghathi	farahsoliman9490@gmail.com	Ankara University
Fernanda Rodrigues	fernanda.rodrigues@student.uc.pt	University of Coimbra
Filomena Lelario	filomena.lelario@unibas.it	University of Basilicata
Flavia Melati Chiappara	flavia.melatichiappara2@mail.dcu.ie	Dublin City University
Gianluca Li Puma	gianluca.lipuma@unipa.it	University of Palermo (UNIPA)
Giuliana Bianco	giuliana.bianco@unibas.it	University of Basilicata

Name	Email	Institution
Grazia Accoto	grazia.accoto@arpab.it	ARPA Basilicata
Guilherme Ferreira Pinto	guilhermepinto@ua.pt	Universidade de Aveiro
Hongyan Chen	honche@ceh.ac.uk	UK Centre for Ecology & Hydrology
Hugo Filipe Margaça Rocha	hugofmr@ua.pt	Universidade de Aveiro
Igor Emanuel Zenha de Oliveira	igor.zenha.oliveira@gmail.com	Faculdade de Farmácia da Universidade do Porto
Inês Quintela	up202006309@up.pt	FEUP
Isabel Paula Lopes Brás	ipbras@estgv.ipv.pt	IPV-ESTGV
Joana Bastos Batista	jba.batista@campus.fct.unl.pt	NOVA FCT
Joana Filipa Monteiro de Sousa	uc2011141774@student.uc.pt	Universidade de Coimbra
Joanna Dołżonek	joanna.dolzonek@ug.edu.pl	University of Gdańsk
João Filipe Rodrigues	jsrodrigues@hovione.com	HOVIONE FARMACIÊNCIA SA
Joaquin Alberto Pereira Marrero	Up201604408@fe.up.pt	FEUP
Katrzyna Pilat	katarzyna.pilat@arpab.it	ARPAB
Leonor Cardielos dos Reis Barroca	lcbarroca@fe.up.pt	FEUP
Lucélia Hoehne	luceliah@univates.br	Univates
Lucia De Marchi	lucia.demarchi@unipi.it	University of Pisa
Magda Caban	magda.caban@ug.edu.pl	University of Gdansk
Manuel Loureiro	manuel.loureiro@hamamatsu.eu	Hamamatsu Photonics
Maria Fernanda Fontoura Nogueira	welcome2maria@gmail.com	Instituto Superior de Engenharia do Porto
Maria Goreti Carvalho Pereira	goreti.pereira@ua.pt	Universidade de Aveiro
Maria Pavlaki	maria.pavlaki@ua.pt	University of Aveiro
Merve Yence	merve.yence@gmail.com	Lokman Hekim University
Namrata Ravindra Patil	namratapatil7767@gmail.com	SRM UNIVERSITY AP
Paola Verlicchi	paola.verlicchi@unife.it	University of Ferrara
Paulo Miguel Soares de Sousa	up201206729@edu.fe.up.pt	FEUP
Pedro Miguel Cruz Matias	petermatias1998@gmail.com	Universidade de Coimbra
Ricardo Malheiro	readytopub@gmail.com	ReadyToPub - Author Services Provider
Rita Certo Gomes Gouveia	ritacggouveia@ua.pt	Universidade de Aveiro
Robert Peeling	r.p@britest.co.uk	Britest Ltd
Rosa Freitas	rosafreitas@ua.pt	University of Aveiro
Royston Jerome Colaso	roystonjeromecolaso@gmail.com	SRM UNIVERSITY AP
Rudolf J. Schneider	rudolf.schneider@bam.de	BAM Federal Institute for Materials Research and Testing
Sibel A. Ozkan	ozkan@pharmacy.ankara.edu.tr	Ankara University
Sofia Camila Walzer	sofia.walzer@kaust.edu.sa	King Abdullah University of Science and Technology
Solange Carolina Caniço Fernandes	sfernandes@hovione.com	Hovione
Susana Patrícia Mendes Loureiro	sloureiro@ua.pt	University of Aveiro
Tess Goessens	tess.goessens@ugent.be	Ghent University
Tiago Fernando Teixeira Morais	tiagomorais@ua.pt	Universidade de Aveiro
Valentina Guimarães da Silva	valentinagsilva@ua.pt	Universidade de Aveiro
Vanessa Maybruck	vanessa.maybruck@colorado.edu	University of Colorado Boulder
Valdemar Inocêncio Esteves	valdemar@ua.pt	University of Aveiro
Vânia Maria Amaro Calisto	vania.calisto@ua.pt	Universidade de Aveiro & CESAM
Yolanda Valcarcel Rivera	yolanda.valcarcel@urjc.es	Rey Juan Carlos University
Zélia Rosa da Silva Barbosa Moreira	zeliabarbosa@estesc.ipc.pt	IPC-ESTeSCoimbra



Recognizing Innovation



Winners for the 11th Award (2024)



Creativity Prize

[1] The team of Maria Cristina Rulli (Polytechnic of Milan, Italy) and Paolo D'Odorico (University of California,

freshwater stewardship in a changing, globalised world.

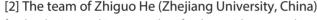




Maria Cristina Rulli







for developing working, versatile soft robots with unprecedented manoeuvrability that have the capacity for numerous underwater research and monitoring applications. Team members include: Pengcheng Jiao and Yang Yang.



Surface Water Prize

Qiuhua Liang (Loughborough University, UK) and his team

for developing innovative, open-source, multi-GPU hydrodynamic models to support realtime flood forecasting at high temporal-spatial resolutions. Team members include: Huili Chen, Xiaodong Ming, Xilin Xia, Yan Xiong and Jiaheng Zhao.



Oiuhua Liang



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.





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.





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.



Invitation for Nominations 12th Award (2026)

Nominations open online until 31 December 2025 www.psipw.org e-mail: info@psipw.org