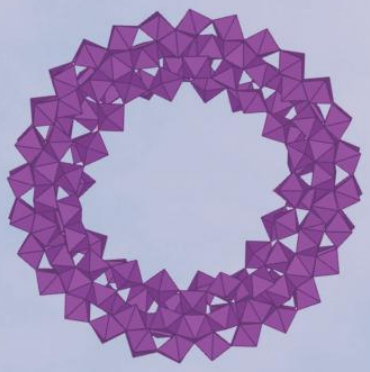
2026 IBiCC

15th Inorganic & Bioinorganic Chemistry Conference



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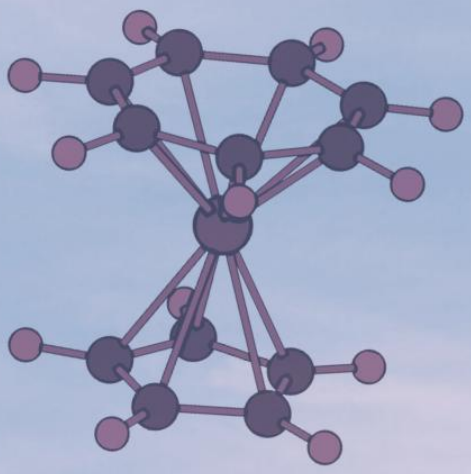
Faculdade de Ciências

8 - 10th April 2026



BOOK OF ABSTRACTS

15th Inorganic & Bioinorganic Chemistry Conference (15th IBiCC)

Faculty of Sciences, University of Lisbon, Portugal

8 – 10 April 2026

Editors

Carla D. Nunes

Nuno Bandeira

Tânia S. Morais

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Sociedade Portuguesa de Química

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WELCOME

It is our great pleasure and honor to welcome you to the 15th Inorganic & Bioinorganic Chemistry Conference (15th IBiCC), organized by the Division of Inorganic and Bioinorganic Chemistry of the Portuguese Chemical Society (SPQ) in collaboration with the Faculdade de Ciências da Universidade de Lisboa.

This 15th edition of IBiCC provides a valuable platform for academic scientists and researchers to share their latest results, exchange ideas, and foster collaborations across the various fields of Inorganic Chemistry. The conference highlights key thematic areas including Coordination and Supramolecular Chemistry, Catalysis, Magnetochemistry, Energy and Photochemistry, Bioinorganic Chemistry, Inorganic Materials and Nanoparticles, Nuclear Chemistry, and Theoretical Inorganic Chemistry.

We wish you an inspiring and scientifically enriching meeting, and hope that discussions and contacts during 15th IBiCC 2026 will contribute to new insights and fruitful collaborations.

On behalf of the Organizing Committee,

Welcome to Lisbon

Yours sincerely,

Carla D. Nunes

Chair of the 15th IBiCC

President of the SPQ Division of Inorganic and Bioinorganic Chemistry

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ACKNOWLEDGMENTS AND SPONSORS

Institutional support

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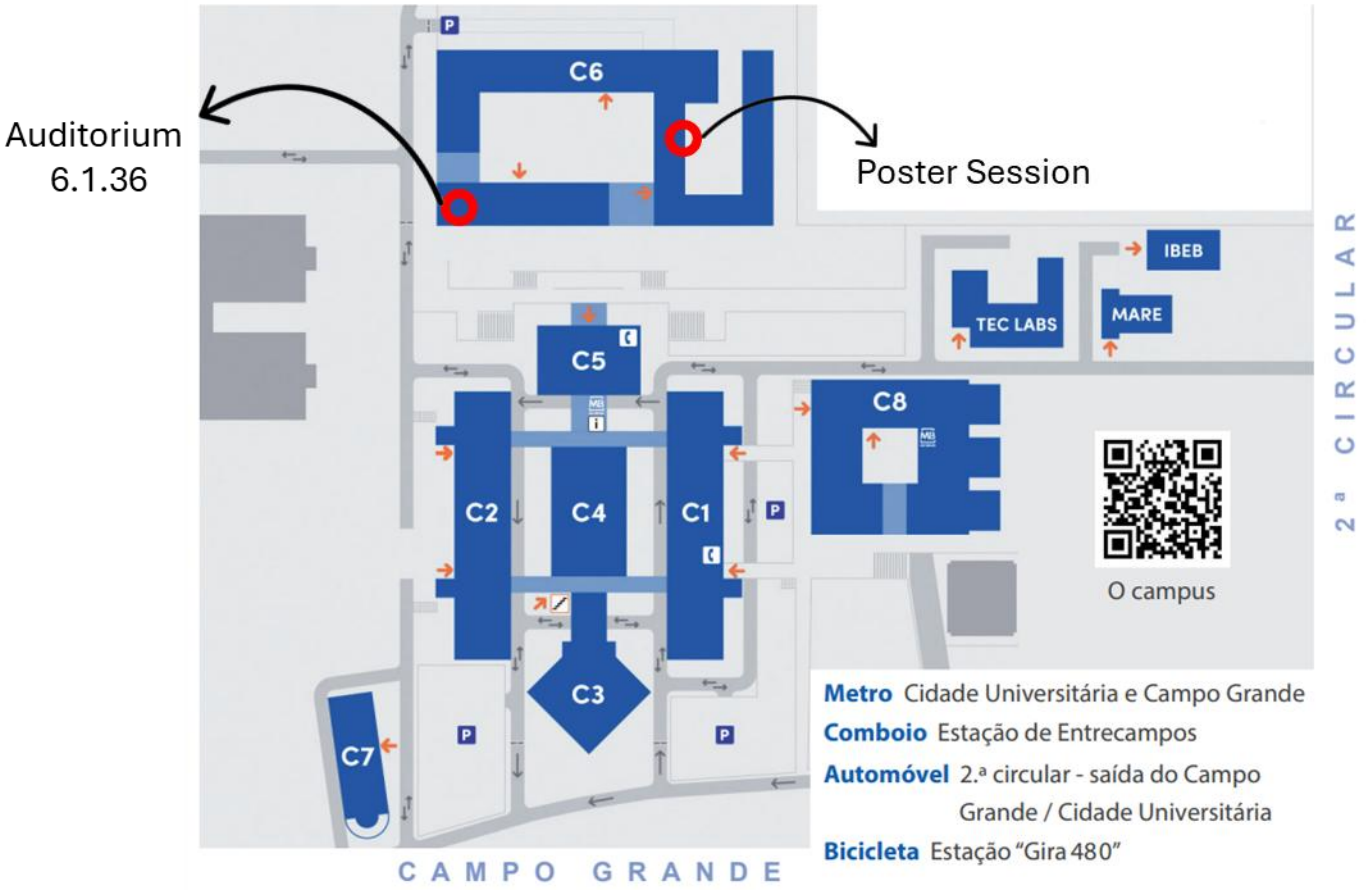
GENERAL INFORMATION

Venue

Faculty of Sciences of the University of Lisbon (FCUL), Building C6.

Campo Grande, 1749-016 Lisboa, Portugal.

The FCUL campus is located in Campo Grande and is easily accessible by public transport.



Registration

All attendees must register at the registration/information desk located at the entrance of C6 Bd that will be open from Wednesday 12h00 through the course of the scientific program.

Audio-visual equipment

The conference room is equipped with a computer and standard audio-visual equipment, namely a data projector, projection screen and laser pointer. Each speaker should upload and review his/her presentation as far in advance as possible, being advised for it to be placed in the previous session. Please take note of the following:

All presentations must use a PowerPoint (Microsoft) or PDF format. A USB memory stick should be used for uploading the presentation. Personal laptops cannot be used for presentations.

Communications

Plenary Lectures (PL) will last 50+10 min, Keynote Lectures (KL) will last 30+10, Invited Lectures 15+5 min and Oral Communications 12+5 min, including discussion.
All speakers are requested to carefully plan the presentation in order to respect the schedule, avoiding delays in the program.
The Book of Abstracts is organized alphabetically by the last name of the presenting author.

Poster sessions

Posters should be put upon registration and remain displayed in the stands throughout the scientific program. Members of the organizing committee will be available to assist attendees during poster set-up. Posters should be taken it down by the end of the closing session.

Lunch and coffee-break

Lunches are included and will be held near poster stands. Morning and afternoon sessions will be interrupted for Coffee-Break, which are also held simultaneously with Poster Session.

Social event

The Conference dinner will be held at Restaurante Jardim da Luz on April 9th at 20h30.
Largo da Luz – Quartel da Formação Carnide
1600-498 Lisboa
http://jardimdaluz.pt

PROGRAM

	Wednesday, April 8	Thursday, April 9	Friday, April 10
09:00 – 09:20		PL2 Peter-Leon Hagedoorn	KN6 Andreia Peixoto
09:20 – 09:40			
09:40 – 10:00			IL5 - Ana Margarida Silva
10:00 – 10:20		IL1 - Oscar Rojas	IL6 - Ana Daniel-da-Silva
10:20 – 10:40		OC1 - Sara M. A. Pinto OC2 – M. Paula Robalo	KN7 Ana Petronilho
10:40 – 11:00			
11:00 – 11:20		Coffee Break	Coffee Break
11:20 – 11:40			
11:40 – 12:00		KN3 Filipe Folgosa	OC6 - Ana C. Fernandes OC7 - Sandra Gago OC8 -Tito Trindade
12:00 – 12:20	**Registration**		
12:20 – 12:40		IL2 - Tiago Cruz	
12:40 – 13:00		Group Photo	IL7 – Leonor Morgado
13:00 – 13:20			Lunch & Poster Session
13:20 – 13:40		Lunch & Poster Session	
13:40 – 14:00	Opening Ceremony		
14:00 – 14:20		KN4 Beatriz Royo	IL8 – Adriana Pinheiro
14:20 – 14:40			OC9 - Inês Cardoso Pereira OC10 – Marco Sá OC11 - Clara Rodrigues Pereira
14:40 – 15:00		IL3 - Maria João Ferreira	
15:00 – 15:20	PL1 Karl Kirchner	IL4 - Luis Cunha Silva	
15:20 – 15:40		OC3 – Nuno Bandeira OC4 - Célia Romão	KN8 Paulo J. Costa
15:40 – 16:00			
16:00 – 16:20	KL1 Luisa Martins	Coffee Break	Coffee Break
16:20 – 16:40			
16:40 – 17:00	KL2 Rui Carrilho	OC5 - Manuel Aureliano	Award Alberto Romão Dias Pedro Teixeira Gomes
17:00 – 17:20		KN5 M. Dulce Belo	
17:20 – 17:40	Welcome Reception		
17:40 – 18:00		Division Meeting	Closing Session
18:00 – 18:20			
18:20 – 18:40			

20:30 – 23:00		**Congress Dinner**	

DETAILED PROGRAM

Wednesday, April 8	
14:00	Opening Ceremony **Conceição Freitas**, *Diretora da Faculdade de Ciências, FCUL* **Jorge Parola**, *Secretário-Geral da Sociedade Portuguesa de Química* **José Manuel Nogueira**, *Presidente Departamento Química e Bioquímica, FCUL* **Carla D. Nunes**, *Presidente Divisão Química Inorgânica e Bioinorgânica, FCUL*
	Session Chair Maria José Calhorda and Isabel Moura
15:00	Plenary Lecture 1 **Karl Kirchner**, *Technical University Vienna* Mn(I) and Fe(II) Complexes involving E-H (E = H, C, Si, B) Bond Activation Reactions
16:00	Keynote Lecture 1 **Luísa Martins**, *Instituto Superior Técnico* Unlocking catalytic potential with C-scorpionate metal complexes
16:40	Keynote Lecture 2 **Rui Carrilho**, *Universidade de Coimbra* Biochar-based catalysis at the crossroads: sustainable activation of CO and CO_2 toward value-added molecules
17:20	**Welcome Reception**

Thursday, April 9	
	Session Chair José Moura
09:00	Plenary Lecture 2 **Peter-Leon Hagedoorn**, *Delft University of Technology* Exploring the mechanism of metalloenzymes using Microsecond timescale rapid mixing techniques
10:00	Invited Lecture 1 **Oscar Rojas**, *ITQB-NOVA* Ruthenium-arene complexes as a modular platform for anticancer drug development
10:20	Oral Communication 1 **Sara M. A. Pinto**, *Universidade de Coimbra* Development of manganese porphyrins as redox-sensitive MRI contrast agents
10:40	Oral Communication 2 **M. Paula Robalo**, *ISEL-Instituto Superior de Engenharia de Lisboa* Rapid microwave-assisted synthesis of benchmark Iron(II) complexes
11:00	Coffee Break
	Session Chair Inês Cardoso Pereira
11:40	Keynote Lecture 3 **Filipe Folgosa**, *ITQB-NOVA* Elucidating redox-linked structural dynamics in e. Coli no reductase flavodiiron protein's active site

12:20	**Invited Lecture 2** **Tiago F. C. Cruz**, *Institute of Applied Synthetic Chemistry, TU Wien* Enhancing catalytic activity by including boranes in the secondary coordination sphere of transition metal complexes
12:40	Group Photo Lunch & Poster Session
	Session Chair Isabel Moura
14:00	**Keynote Lecture 4** **Beatriz Royo**, *ITQB-NOVA* Beyond noble metals: cooperative manganese and molybdenum catalysis driven by bis-triazolylidene ligands
14:40	**Invited Lecture 3** **Maria João Ferreira**, *IST-ID* Titanium-catalyzed synthesis of ureas
15:00	**Invited Lecture 4** **Luís Cunha-Silva**, *LNEG - Laboratório Nacional de Energia e Geologia* One-step fabrication of MOF-based mixed matrix Membranes: sustainable energy-related processes
15:20	**Oral Communication 3** **Nuno A. G. Bandeira**, *BioISI* The perferrate puzzle: the challenge of extreme oxidation states in theoretical chemistry
15:40	**Oral Communication 4** **Célia V. Romão**, *Faculdade de Ciências, ULisboa* Metal-induced biofilm formation in Deinococcus radiodurans
16:00	Coffee Break
	Session Chair Clara Gomes
16:40	**Oral Communication 5** **Manuel Aureliano**, *Universidade do Algarve* Polyoxovanadates with anti-breast cancer activity and effects in g-actin polymerization
17:00	**Keynote Lecture 5** **Dulce Belo**, *Instituto Superior Técnico* One molecular motif, many functions: transition metal bisdithiolene complexes, from flexible electronics to cancer therapy
17:40	Division Meeting

Friday, April 10	
	Session Chair Cristina Freire
09:00	**Keynote Lecture 6** **Andreia F. Peixoto**, *LAQV-REQUIMTE, FCUP* Closing the loop: from biomass to bioactive molecules and functional catalytic materials
09:40	**Invited Lecture 5** **Ana Margarida Silva**, *LAQV/REQUIMTE, ICBAS, Universidade do Porto* Metallochlorins: a privileged scaffold for enhanced photodynamic therapy
10:00	**Invited Lecture 6** **Ana Daniel-da-Silva**, *CICECO-Universidade de Aveiro* Designing functional magnetic nanomaterials for Sustainable water purification
10:20	**Keynote Lecture 7** **Ana Petronilho**, ITQB-NOVA Synthesis and applications of metallanucleosides
11:00	Coffee Break
	Session Chair Olinda Monteiro
11:40	**Oral Communication 6** **Ana C. Fernandes**, *IST, Universidade de Lisboa,* Catalytic strategies for plastic waste upcycling: towards a sustainable circular economy
12:00	**Oral Communication 7** **Sandra Gago**, *LAQV-REQUIMTE, FCT NOVA* Metal and carbon-based materials for photocatalytic hydrogen production
12:20	**Oral Communication 8** **Tito Trindade**, *University of Aveiro* Green chemistry routes to perovskite nanocrystals for solar cells
12:40	**Invited Lecture 7** **Leonor Morgado**, *UCIBIO, NOVA FCT* Exploring geobacter inner membrane associated oxidoreductases towards extracellular electron transfer
13:00	Lunch & Poster Session
	Session Chair Beatriz Royo
14:00	**Invited Lecture 8** **Adriana Pinheiro**, *Federal University of Pelotas* Schiff base copper(II) complexes: DNA damage and cellular responses in colorectal cancer cells
14:20	**Oral Communication 9** **Inês Cardoso Pereira**, *ITQB NOVA* Converting CO_2 with a unique tungsten-dependent enzyme
14:40	**Oral Communication 10** **Marco Sá**, *Centro de Química Estrutural, Faculdade de Ciências, ULisboa* FGFR-Targeted ruthenium–peptide conjugates with pH-responsive linkers for selective breast cancer therapy

15:00	**Oral Communication 11** **Clara Rodrigues Pereira**, *LAQV-REQUIMTE, Universidade do Porto* Thermotwin: scalable thermally-chargeable textile supercapacitors based on $MnFe_2O_4$/carbon hybrids
15:20	**Keynote Lecture 8** **Paulo J. Costa**, *BioISI, Faculty of Sciences, University of Lisbon* Bridging chemical complexity with computational chemistry: from coordination complexes to biological systems
16:00	Coffee Break
	Chair Carlos Romão and Joaquim Faria
16:40	**Award Alberto Romão Dias** Pedro Teixeira Gomes, *Instituto Superior Técnico*
17:40	**Clossing Ceremony** **Joaquim Faria**, *Presidente da Sociedade Portuguesa de Química* **Carla D. Nunes**, *Presidente Divisão Química Inorgânica e Bioinorgânica, FCUL*

Plenary Lectures

Exploring the mechanism of metalloenzymes using Microsecond timescale rapid mixing techniques

R.A. Schmitz[a], M. Boll[b], X. Li[c], D. Tischler[d], S. Gao[e], S. Todorovic[f], P.L. Hagedoorn[a]*

[a]Department of Biotechnology, Delft University of Technology, Delft, The Netherlands; [b] Microbiology, Faculty of Biology, Albert-Ludwigs-University Freiburg, Freiburg, Germany; [c] Division of Biology and Chemistry, Paul Scherrer Institute, Villigen, Switzerland; Microbial Biotechnology, [d] Ruhr University Bochum, Bochum, Germany; [e] Tianjin Institute of Industrial Biotechnology, Chinese Academy of Sciences, Tianjin, China; [f] ITQB, Universidade NOVA de Lisboa, Oeiras, Portugal
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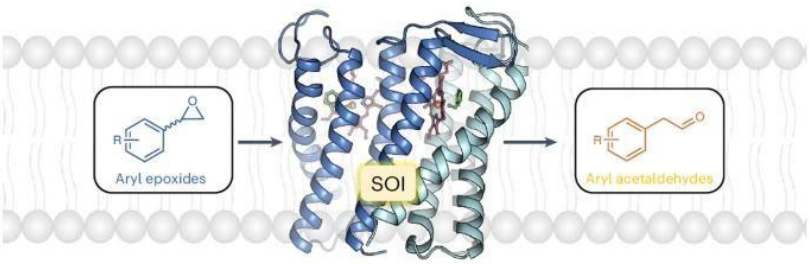
Roughly one third of all enzymes contain one or more metal cofactor, and the identity, oxidation state and coordination environment of the metal cofactor provides essential functional information. EPR spectroscopy is very useful to determine the redox state and obtain information on the direct environment of the metal sites in enzymes. We have explored the mechanism of metalloenzymes using ultrafast mixing and freezing techniques and used EPR spectroscopy to examine enzyme catalytic intermediate states of a heme enzyme chlorite dismutase and a tungsten-cofactor and FeS cluster containing enzyme Benzoyl-coA reductase [1,2]. Furthermore, we have provided direct evidence on the role of a heme cofactor in an unexpected heme enzyme Styrene oxide isomerase (figure) and in a new catalase-family enzyme Chanoclavine synthase which exhibits an unprecedented superoxide mechanism [3,4].



References:
[1] J. Püschmann, et al., ACS Catal. 2021, 11, 14533-14544.
[2] C.S. Seelmann, et al., ACS Catal. 2023, 13, 8631-8641.
[3] B. Khanppnavar, et al., Nat. Chem. 2024, 16, 1496-1504.
[4] C.C. Chen, et al., Nature, 2025, 840-846.

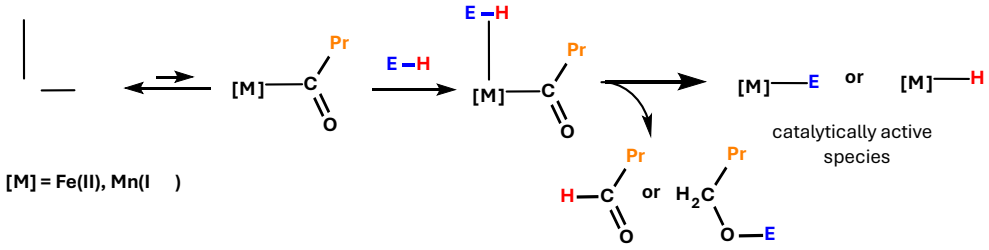
Acknowledgments:
This work was supported by COST (European Cooperation in Science and Technology) Action FeSImmChemNet (CA21115) and funding from the European Union's Horizon Europe research and innovation programme under grant agreement no. 101183014 (project McGEA) and by a grant from the European Union's HORIZON-EIC-2023-PATHFINDEROPEN-01 under grant agreement No 101129798

Mn(I) and Fe(II) Complexes involving E-H (E = H, C, Si, B) Bond Activation Reactions

Karl Kirchner

Institute of Applied Synthetic Chemistry, Technische Universität Wien, Getreidemarkt 9, 1060 Wien, Austria
**karl.kirchner@tuwien.ac.at*

The utilization of base-metal catalysts represents an emerging field in homogeneous catalysis. Among others, manganese-based complexes were proven to be highly competitive catalysts for several (de)hydrogenation reactions.



This lecture outlines the potential of Mn(I)- and Fe(II)-carbonyl alkyl and related complexes for the activation of non-polar and moderately polar E-H (E = H, C, Si, B) bonds and disclose our successful approach for the utilization of complexes in the field of homogeneous catalysis.[1-5] We took advantage of the fact that Mn(I) and Fe(II) alkyl carbonyl complexes undergo migratory insertion of the nucleophilic alkyl ligand into the polarized CO moiety, yielding via a coordinatively unsaturated acyl complex the catalytically active M-E and/or M-H species.

Our investigations unveiled novel insights in reaction pathways of the hydrosilylation and hydroboration of alkenes and alkynes, hydrogenations of alkenes, alkynes, ketones and the selective isomerization of alkenes.

References:
[1] D. P. Zobernig, B. Stöger; L. F. Veiros, K. Kirchner, *ACS Catal.* **2024**, *14*, 12385-12391.
[2] I. Blaha, S. Weber; R. Dülger, L. F. Veiros, K. Kirchner,. *ACS Catal.* **2024**, *14*, 13174-13180.
[3] S. Weber, K. Kirchner, *Acc. Chem. Res.* **2022**, *55*, 2740-2751
[4] S. Weber; D. P. Zobernig, B. Stöger, L- F. Veiros, K. Kirchner, *Angew. Chem., Int. Ed.* **2021**, *60*, 24488-24492.
[5] S. Weber, M. Glavic, B. Stöger, E. Pittenauer, M. Podewitz, L. F. Veiros, K. Kirchner, *J. Am. Chem. Soc.* **2021**, *143*, 17825-17832.

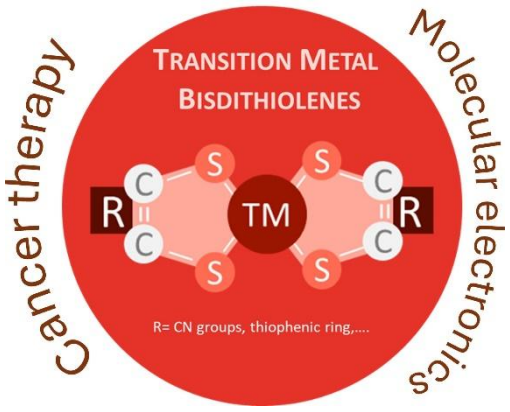
Keynote Lectures

One molecular motif, many functions: transition metal bisdithiolene complexes, from flexible electronics to cancer therapy

Dulce Belo

Department of Nuclear Sciences and Engineering (DECN), Instituto Superior Técnico, Universidade de Lisboa, Instituto de Telecomunicações (IT), Organic Electronics Group, Campus Tecnológico e Nuclear, 2695-066 Bobadela LRS, Portugal
**dbelo@ctn.tecnico.ulisboa.pt*

Transition metal bisdithiolene complexes are a unique class of molecular systems where structural simplicity meets remarkable electronic versatility. Their non-innocent ligands and strong metal–sulfur interactions enable highly delocalized electronic structures, allowing fine tuning of redox properties, conductivity, and spin states. Our work has explored these complexes as platforms for single-component molecular metals (SCMM), where metallic behaviour arises from a single neutral molecule. Through molecular design and control of intermolecular interactions, we have contributed to the development of systems with extended electronic delocalization and 3D transport properties, relevant for flexible and lightweight electronic applications [1]. More recently, we have extended this approach to biomedicine. Gold bisdithiolene complexes show promising activity against ovarian cancer cells, including the ability to overcome cisplatin resistance, likely through modulation of cellular redox pathways rather than direct DNA targeting [2]. These results highlight how the same molecular motif can bridge materials science and biology. This lecture will discuss how electronic structure and molecular design underpin this functional diversity, positioning bisdithiolene complexes as versatile platforms for future technologies and therapeutic strategies.



References:
[1] Mariana F. G. Velho, Rafaela A. L. Silva, Dulce Belo, J. Mater. Chem. C, 2021, 9, 10591.
[2] Dulce Belo, Sandra Rabaça, Sara G Fava, Sílvia A Sousa, Diogo Coelho, Jorge H Leitão, Teresa Pinheiro, Célia Fernandes, Fernanda Marques, Molecules, 2025, 30(15):3270.

Biochar-based catalysis at the crossroads: sustainable activation of CO and CO_2 toward value-added molecules

Rui M. B. Carrilho*[a], Shahab Zomorodbakhsh[a], Beatriz R. Barbosa[a], Mariette M. Pereira[a]

[a] Coimbra Chemistry Centre, Institute of Molecular Sciences (CQC-IMS), Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal
**rui.carrilho@uc.pt*

The development of sustainable catalytic technologies demands renewable materials capable of converting abundant C1 molecules such as CO_2 and CO into value-added chemicals.[1] In this context, biochar, derived from biomass pyrolysis, has emerged as a versatile carbon platform,[2] combining high surface area, tunable porosity, rich surface functionality, and structural robustness, making it suitable both as a catalyst and as a support for metal species. This communication highlights two examples of biochar-based systems for C1 molecules activation (**Figure 1**). Metal-coated biochar nanomaterials, prepared via magnetron sputtering, act as heterogeneous catalysts for the cycloaddition of CO_2 to epoxides, enabling selective formation of cyclic carbonates, and showing good recyclability.[3] Additionally, nitrogen-doped biochar-supported palladium catalysts promote aminocarbonylation of iodoarenes with CO, efficiently affording aryl carboxamides. Aspects of catalytic activity, selectivity and reuse will be discussed, underscoring the potential of biochar as a sustainable and tunable platform bridging biomass valorization and advanced catalytic transformations.

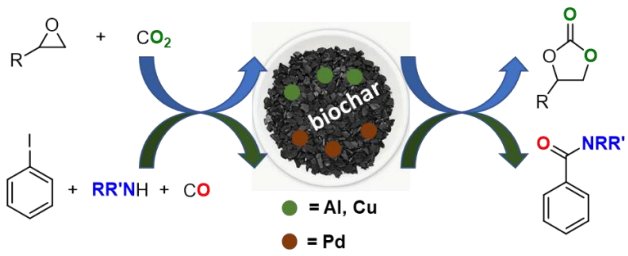


Figure 1. Biochar-based catalysts for C1 molecules transformation into value-added products.

References:

[1] R. M. B. Carrilho, M. J. F. Calvete, G. Mikle, L. Kollár, M. M. Pereira; Chin. J. Chem., 2024, 42, 199–221.
[2] S. Zomorodbakhsh, L. D. Dias, M. J. F. Calvete, A. F. Peixoto, R. M. B. Carrilho, M. M. Pereira; Catalysts, 2025, 15, 568.
[3] S. Zomorodbakhsh, A. C. S. Gonzalez, I. G. Cruz, G. Piccirillo, T. M. R. Maria, I. S. Marques, A. F. Peixoto, J. M. Gil, F. Ferreira, R. M. B. Carrilho; Adv. Sustainable Syst., 2025, 9, 2400431.

Acknowledgments:
This work was supported by Fundação para a Ciência e a Tecnologia (FCT) the European Union (NextGenerationEU) funds through projects UIDB/00313/2025, UID/PRR/00313/2025, UID/PRR2/00313/2025 and LA/P/0056/2020, and by COMPETE2030/FEDER through the EcoxoPlas Project (00882400 - nº 15161).

Bridging chemical complexity with computational chemistry: from coordination complexes to biological systems

Paulo J. Costa *[a]

[a] BioISI - Instituto de Biossistemas e Ciências Integrativas and Departamento de Química e Bioquímica, Faculdade de Ciências Universidade de Lisboa, Lisbon, Portugal
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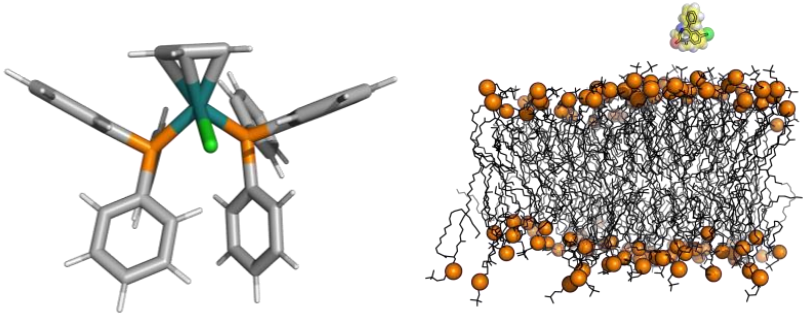
Computational chemistry provides a powerful framework to understand how electronic structure controls reactivity and molecular recognition, from metal-ligand bonds in coordination complexes to weak, directional interactions in complex environments. In this keynote lecture, selected examples of *in silico* approaches applied to organometallic and inorganic systems, and their extension to increasingly complex contexts will be presented. A particular emphasis will be placed on less conventional noncovalent interactions, for which simple and intuitive descriptors, such as those based on the intrinsic bond strength index, can provide fast and reliable estimates of interaction energies [1]. These concepts are further explored in biomolecular environments using molecular dynamics simulations, highlighting the role of such interactions in biological systems [2] and illustrating how chemical concepts extend naturally across increasing levels of complexity.



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[2] R. Nunes, D. Vila-Viçosa, P. J. Costa, J. Am. Chem. Soc., 2021, 143, 11, 4253-4267.

Acknowledgments:
This work was supported by FCT under projects 2024.16247.PEX (PJC; 10.54499/2024.16247.PEX), UID/04046/2025 (BioISI; DOI: 10.54499/UID/04046/2025), and 2023.10475.CPCA (PJC; DOI: 10.54499/2023.10475.CPCA.A2). The Portuguese Recovery and Resilience Plan (PRR) is also acknowledged for the under the FCT-Tenure program(2023.15441.TENURE.008/CP00003/CT00005)

Elucidating redox-linked structural dynamics in e. Coli no reductase flavodiiron protein's active site

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Flavodiiron proteins (FDPs) play a vital role in protecting organisms from nitric oxide and oxygen toxicity by converting these reactive species into the harmless water and nitrous oxide molecules [1]. Despite the well-established nature of the proteinaceous ligands coordinating the diiron active site, its precise coordination environment has remained a subject of debate. To resolve these structural uncertainties, we utilized ^{57}Fe Nuclear Resonance Vibrational Spectroscopy, together with Mössbauer spectroscopy, Electron Paramagnetic Resonance and Density Functional Theory to elucidate the redox-linked structural dynamics of the FDP from *Escherichia coli*. Our investigation reveals that the as-isolated diferric state consists of a dihydroxo-bridged Fe(III)-(μOH^-)$_2$-Fe(III) center, which, upon reduction, undergoes a specific rearrangement to a monohydroxo Fe(II)-(μOH^-)-Fe(II) one, through the loss of one bridging ligand [2]. One of the hydroxo bridges in the as-isolated, oxidized, state had remained undetected in previous X-ray studies [3]. These findings provide a robust framework for interpreting ligand dynamics and catalytic mechanisms in diiron enzymes. Given that diiron active sites are ubiquitous in other enzyme classes, these insights into metalloenzyme dynamics have broad implications across the field of bioinorganic chemistry.

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Unlocking catalytic potential with C-scorpionate metal complexes

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Catalysis is one of the most important and pervasive technologies in the chemical industry, with profound societal and economic impact, yet the development of more effective catalysts and new catalytic processes remains a critical challenge.

Bio-inspired C-scorpionate metal complexes have unlocked an exciting array of catalytic applications, namely in challenging reactions of industrial significance [1]. Herein the successful catalytic strategies for using inert carbon dioxide or alkanes as carbon feedstock for the syntheses of functionalized added-value organic compounds, as well as for lignin biomass valorization, are addressed.

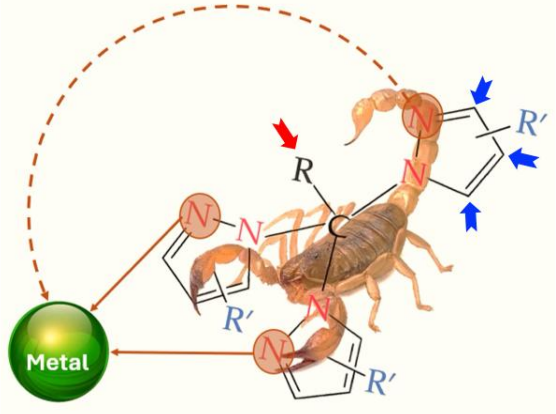

Figure 1 – Coordination of a C-scorpionate tris(1H-pyrazol-1-yl)methane compound to a metal center and comparison with a scorpion attack to its prey. Highlighted are the functionalization sites of the C-scorpionate compound.

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Closing the loop: from biomass to bioactive molecules and functional catalytic materials

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The transition towards a circular and sustainable economy requires innovative strategies to transform renewable resources and waste streams into high-value products. In this context, biomass and bio-residues represent abundant and largely underexploited feedstocks that can serve as versatile platforms for the production of bioactive molecules, advanced functional materials, and sustainable catalysts.[1,2]

In this keynote, recent advances in catalytic and biorefinery approaches for the valorisation of biomass-derived resources will be presented. Focus will be given to how integrated processes can contribute to “closing the loop” within circular chemical systems. Special emphasis will be placed on the transformation of marine bio-residues, particularly shrimp shells, into bioactive compounds, valuable chemicals, and multifunctional carbon-based materials.

Through the application of green extraction technologies and sustainable catalytic methodologies, these resources can be converted into bioactive ingredients with potential applications in cosmetics, health, and materials science.[3] In parallel, biomass-derived carbon materials, including metal- and heteroatom-doped biochars, have been explored as promising platforms for the development of efficient (electro)catalysts for energy conversion and biomass upgrading.[4]

Overall, a biorefinery concept has been developed that combines green chemistry, catalysis, and biomass valorisation strategies to promote circular processes, transforming waste into valuable resources.

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Synthesis and applications of metallanucleosides

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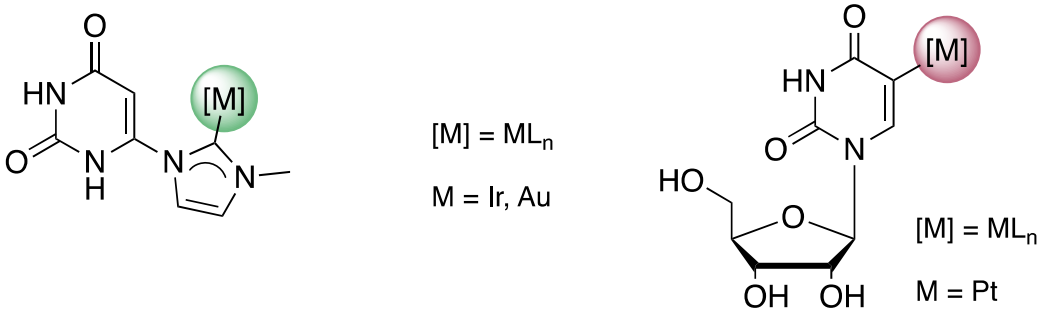
The utilization of ligands based on biologically-relevant compounds has raised interest over the last decades. The main reason for this is the propensity of these ligands to provide access to more selective drugs, due either to a more favorable solubility in physiological media or a higher biocompatibility inside the cells. Modified nucleobases and nucleosides are especially relevant in this context due to their active role as antimetabolites, with widespread medicinal applications.
We have worked in the development of novel nucleosides and nucleobases, modified with metal, aiming to explore their combined effect in medicinal applications. We reported the synthesis of platinum complexes based on guanosine and adenosine, by means of C-X oxidative addition to Pt(0) precursors. More recently, we have focused our attention on synthesis of organometallic nucleosides based on pyrimidines, which are widely employed in the clinic (e.g. 5-Fluorouracil). These metallated nucleosides were subsequently evaluated for their biological activity and these results will be discussed in this communication.



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Beyond noble metals: cooperative manganese and molybdenum catalysis driven by bis-triazolylidene ligands

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Mesoionic 1,2,3-triazolylidene ligands are a prominent class of ligands in organometallic chemistry and catalysis valued for their modular synthesis, their exceptional donor properties, and their ability to act as electron reservoir ligands in redox transformations. Although numerous metal complexes bearing 1,2,3-triazolylidenes have been reported, bidentate systems featuring a methylene bridge between the two triazolylidene units are very rare. In this seminar, we present our recent work on complexes of inexpensive metals supported by such ligands. We describe the synthesis and characterization of new manganese, molybdenum, and tungsten complexes, and their application in borrowing hydrogen and acceptorless dehydrogenative catalysis. Notably, we demonstrate for the first time that methylene-bridged bis(1,2,3-triazolylidene) ligands exhibit genuine metal–ligand cooperation (Figure 1).[1] Reversible deprotonation of the methylene linker generates the active metal species, revealing a non-innocent, proton responsive site that enables new catalytic pathways and expands the design principles of base-metal catalysis.

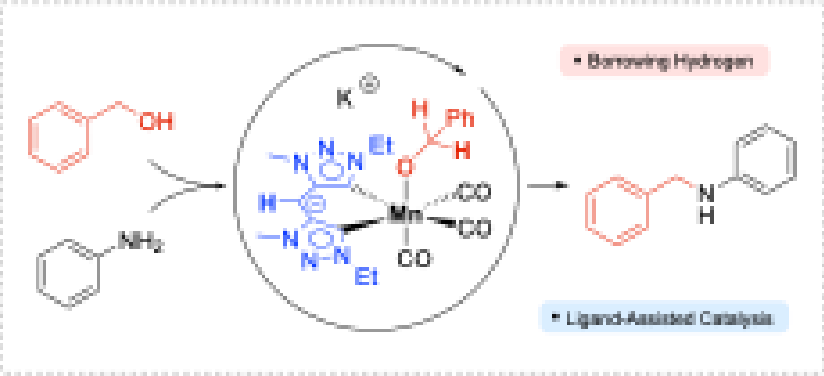

Figure 1. Metal-ligand cooperation in Mn catalysis enabled by non-innocent triazolylidenes

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Invited Lectures

Enhancing catalytic activity by including boranes in the secondary coordination sphere of transition metal complexes

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Ligand design in coordination chemistry is critical in homogeneous catalysis because it regulates the reactivity between the intermediates with the substrates and products. While the primary coordination sphere of a metal center is crucial to catalytic activity and selectivity, outer sphere effects are well-known, for instance in carbonyl group hydrogenations.[1] Thus, manipulation of secondary coordination spheres of metal complexes has proved useful in catalysis.[2] One way of achieving this is to include Lewis acids in the vicinity of a complex. The formation of Lewis pairs between the primary and secondary coordination spheres gives rise to push-pull[3] or substrate directing effects,[4] which kinetically stabilize the reaction intermediates, thus increasing the catalytic activity.

We have been exploring the manipulation of the second coordination sphere of transition metal complexes by incorporating pendant Lewis acidic boranes. When applied in homogeneous catalysis, depending on the type of reaction, the borane-tethered complexes promote the formation of Lewis pairs between the pending borane and the coligands or substrates during catalysis, leading to an enhancement of the catalytic activity, in comparison with the unfunctionalized complexes.

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Titanium-catalyzed synthesis of ureas

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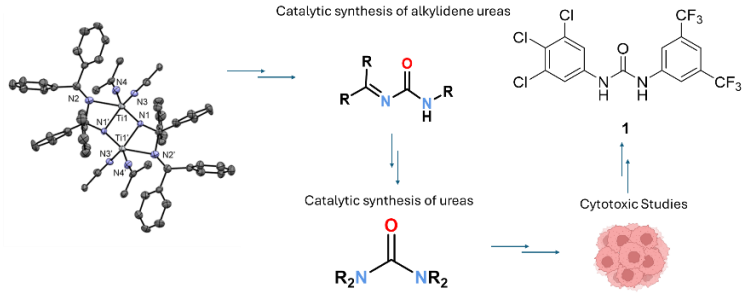
Ketimide ligands have long been recognized as supporting ligands for early transition metals.[1-2] Generally considered spectator ligands, they have occasionally display non-innocent behavior, stabilizing uncommon metal oxidation states.[3] We report herein new Ti complexes supported by $N{=}CAr_2$ ligands that exhibit unusual reactivity: the nitrogen lone pair can attack the carbon atom of an isocyanate. While similar reactivity has previously been observed for Th complexes,[4] we have taken it further: we describe here the unprecedented catalytic synthesis of alkylidene ureas using commercially available $Ti(NMe_2)_4$ as a precatalyst. This methodology can be extended to the synthesis of ureas.

Ureas are valuable compounds with broad applications in industry, agrochemistry, dyes, and pharmacology.[5] All synthesized ureas and alkylidene ureas were evaluated for cytotoxicity against Jurkat, MCF-7, and HEK-293 cell lines. Compound **1** is the most promising candidate demonstrating selectivity towards cancer cell lines (IC_{50} of 0.49 ± 0.1 μM and 2.23 ± 0.34 μM for MCF-7 and Jurkat, respectively *vs*. 4.85 ± 2.21 μM for non-cancerous HEK-293).



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Exploring *geobacter* inner membrane associated oxidoreductases towards extracellular electron transfer

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Geobacter sulfurreducens is the reference model organism for studying extracellular electron transfer in electroactive bacteria. In this process, inner membrane oxidoreductases play a crucial role by linking cytoplasmic metabolism to the periplasmic electron transfer network. The *G. sulfurreducens* genome encodes at least six inner membrane oxidoreductase gene clusters: the cytochrome ImcH, four Cbc complexes containing *b*- and *c*-type heme groups (Cbc3/CbcVWX, Cbc4/CbcSTU, Cbc5/CbcEDCBA, and Cbc6/CbcMNOPQR), and one singleprotein Cbc (CbcL) [1,2]. Among these, ImcH, CbcL, and CbcBA have been implicated in distinct extracellular electron transfer routes: ImcH in routes using high-potential electron acceptors such as Fe(III) chelates, CbcL for low-potential electron acceptors such as Fe(III) oxides (down to −210 mV), and CbcBA at even lower potentials (down to −280 mV) [2]. The periplasmic domain of CbcL (9 *c*-type hemes) and ImcH (7 *c*-type hemes) were the first to be biochemically characterized *in vitro* [3,4], revealing similar midpoint reduction potentials; however, ImcH displays a larger redox-active window despite having fewer heme groups. More recently, we characterized CbcS (4 hemes) [5] and CbcA (7 hemes) [6], which exhibited the highest and lowest midpoint reduction potential values among the four inner membrane oxidoreductases, respectively. Notably, all four oxidoreductases were able to transfer electrons to PpcA, the most abundant triheme cytochrome in the periplasm.

In addition, CbcA crystal structure was determined [6] and compared with AlphaFold structural models of the other inner membrane oxidoreductases, revealing a high degree of structural similarity in heme arrangement.

The biochemical and structural characterization of these oxidoreductases will be presented and discussed in the context of *G. sulfurreducens* electron transfer pathways.

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Schiff base copper(ii) complexes: DNA damage and cellular responses in colorectal cancer cells

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Colorectal cancer (CRC) remains a major global health challenge. Although oxaliplatinbased chemotherapy is widely used, its effectiveness is limited by toxicity and the development of resistance [1]. In this context, copper complexes have emerged as promising metallopharmaceuticals, owing to their redox activity, interactions with biomolecules, and ability to induce oxidative stress and copper-dependent cell death pathways, such as cuproptosis [2]. In this study, we synthesized two novel Cu(II) complexes bearing a tridentate N,N,O Schiff base ligand: complexes **2a** and **2b** (**Figure 1**). These ligands are built upon an invariant quinoline-based Schiff base scaffold, with structural variation introduced at the aldehyde-derived phenolic fragment, which coordinates to Cu(II) the tert-butyl-substituted phenolate (2a) or a naphtholate unit (2b). The complexes were characterized using a combination of physicochemical techniques and computational methods, including density functional theory (DFT), to elucidate their coordination geometry and electronic structure.

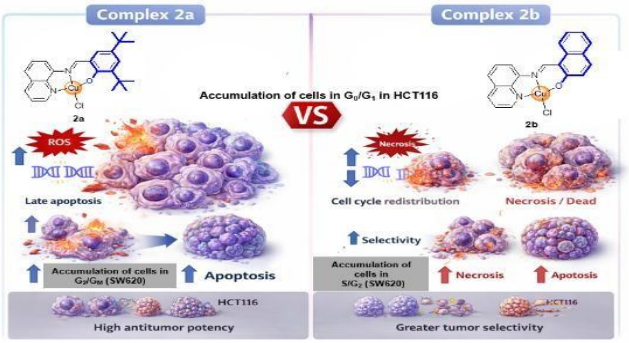

Figure 1. Comparative representation of the cellular mechanisms triggered by the copper complexes **2a** and **2b** in HCT116 cells, highlighting differences in cell death profiles, stress response pathways, and their relative impact on antitumor potency and tumor selectivity. The schematic illustration was generated using Microsoft Copilot.

Biological evaluation in CRC cell lines (HCT116 and SW620) and normal fibroblasts (MRC-5) revealed that coordination to Cu(II) consistently enhanced cytotoxic and antiproliferative effects compared to the free ligands. **2a** exhibited the highest antitumor potency, particularly in HCT116 cells. **2b** displayed moderate cytotoxicity but greater tumor selectivity. Further studies on chemical speciation and DNA repair modulation are warranted to elucidate the active Cu(II) species, better understand cellular recovery pathways, and support the rational optimization of these complexes as therapeutic candidates.

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Ruthenium-arene complexes as a modular platform for anticancer drug development

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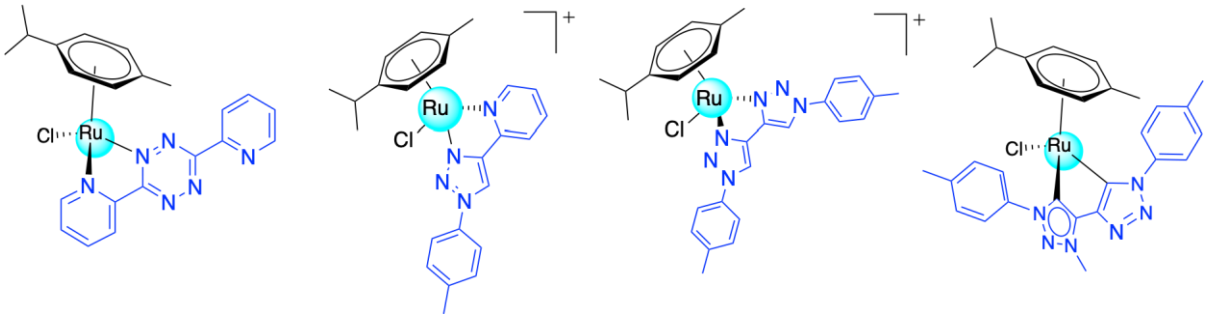
Cancer remains a leading cause of mortality worldwide. Although platinum-based drugs revolutionized chemotherapy, their clinical efficacy is limited by systematic toxicity, acquired resistance, and poor selectivity.[1] The development of new metal-based therapeutic platforms is therefore urgently needed. Ruthenium complexes have emerged as promising alternatives due to their favorable biological properties and demonstrated anticancer activity.[1-3]
A key challenge in drug development is the identification of modular scaffolds capable of accessing broad chemical space. In this context, we investigate ruthenium-arene complexes as a versatile anticancer platform. Our approach evolved from Ru(II) *N,N*-pyridine derivatives to triazole-based systems and ultimately to triazolylidene *N*-heterocyclic carbene complexes, progressively increasing structural diversity while preserving the ruthenium-arene core.[1-3]
The biological performance of these compounds was assessed through comprehensive *in vitro* cytotoxicity studies and *in vivo* validation using zebrafish xenograft models, demonstrating their significant therapeutic potential.



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Designing functional magnetic nanomaterials for sustainable water purification

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The increasing complexity of water contamination scenarios demands the development of advanced remediation materials combining high efficiency, selective pollutant interaction, operational simplicity, and sustainability. In this context, functional magnetic nanomaterials have emerged as highly promising inorganic platforms due to their tunable composition, surface reactivity, and facile magnetic recovery. [1] Such materials also allow the integration of multiple functionalities within a single platform, thereby expanding their potential for advanced water treatment applications. This lecture will present recent advances in the rational design of magnetic nanomaterials for sustainable water purification, with particular emphasis on the relationship between composition, interfacial properties, and performance. Attention will be given to strategies based on surface engineering and hybridization with biopolymers and inorganic components to modulate surface charge, adsorption affinity, and structural robustness in aqueous media. Such approaches provide opportunities to enhance pollutant removal efficiency while broadening the scope of application of these materials. [2,3] Selected case studies will illustrate how the careful control of nanomaterial interfaces and functionality can improve removal performance, recyclability, and process sustainability.

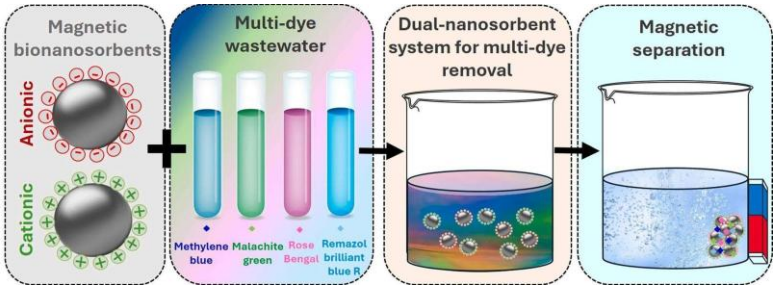

Figure 1. Magnetic bionanosorbents for multi-dye wastewater treatment. [3]

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Metallochlorins: a privileged scaffold for enhanced photodynamic therapy

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Photodynamic therapy (PDT) uses light, molecular oxygen, and a photosensitizer to generate reactive oxygen species (ROS) that can damage target cells, offering a therapeutic approach for cancer and infectious diseases [1]. Recent advancements in PDT involve developing new photosensitizers and genetically engineering conjugates to enhance ROS production and explore cellular signaling [1].

In this study, we synthesized and characterized a series of metallochlorins, assessing their singlet oxygen generation (Fig. 1). The research aims to investigate how metal ions, including Zn(II), Cu(II), Fe(III), Pd(II), Pt(II), influence chlorin structure and properties, specifically the Q band in electronic spectra, spin-orbit coupling efficiency and triplet state stability, which are critical for determining the efficacy of a photosensitizer. The metallochlorins were synthesized via 1,3-dipolar cycloadditions and metallations using conventional, microwave, and/or ohmic heating, with their respective advantages and limitations to be discussed [2, 3].

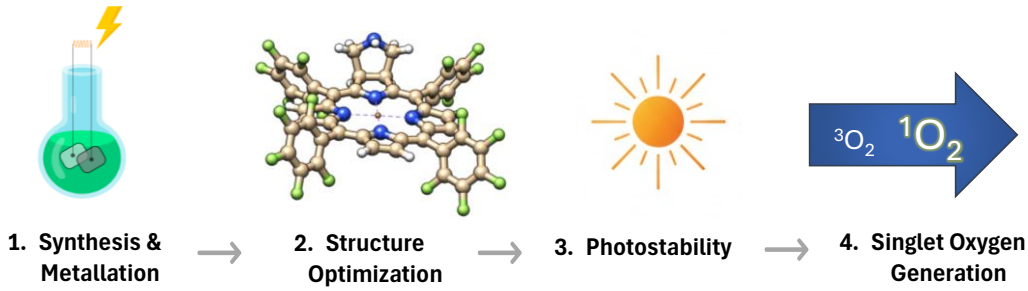

Fig 1. Structure of metallochlorins aiming PDT

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One-step fabrication of mof-based mixed matrix membranes: sustainable energy-related processes

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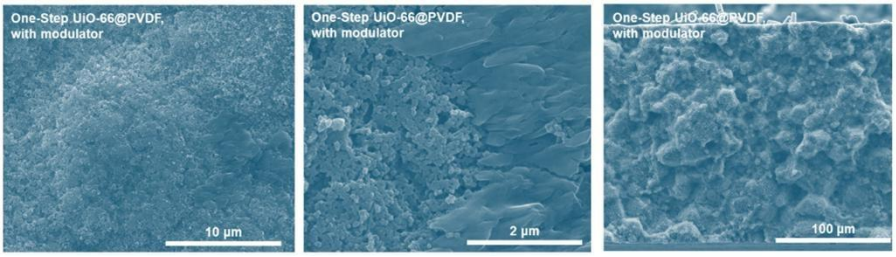
Membrane technology has garnered significant attention across various fields due to its versatility and broad industrial applicability (fuel cells, drug delivery systems, water purification, and gas separation processes, particularly in the context of carbon capture and utilization). Mixed-Matrix Membranes (MMMs), which combine polymer matrices with inorganic fillers, were developed to address some of the limitations of traditional polymer membranes, and the use of catalytically active inorganic fillers in MMMs opens up new opportunities in catalytic process engineering, mitigating issues such as catalyst deactivation and material loss during recovery, making MMMs highly attractive for diverse catalytic processes.

In the research work herein reported, MMM with either pristine or defective UiO-66 Metal–Organic Framework (MOF) fillers were fabricated via a novel one step process. On top of a simpler, more sustainable preparation, these MMMs also exhibit improved catalytic performance for a sulfur oxidation reaction when compared to those produced by the traditional filler dispersion process.[1] Remarkably, this new method for the preparation of functional MMMs was validated for various MOF materials, in addition to the UiO-66 family, opening excellent prospects for the use of these membranes in other applications, particularly as electrocatalysts in reactions related to the production and storage of clean energy.



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Acknowledgments:

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Oral Communications

Polyoxovanadates with anti-breast cancer activity and effects in g-actin polymerization

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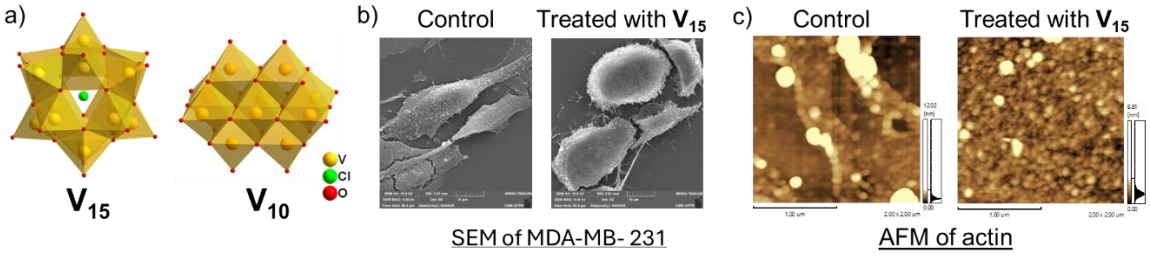
Polyoxovanadates (POVs) interact with a range of proteins and hold potential for breast cancer therapy. G-Actin and F-actin are the globular and filamentous forms of actin, essential for maintaining the cytoskeleton, defining cell shape, and facilitating cell division. In the present work, we demonstrate that decavanadate, $(H_xV_{10}O_{28})^{(6-x)-}$, **$V_{10}$**, and pentadecavanadate, $[(CH_3)_4N]_6[V^{IV}_8V^{V}_7O_{36}Cl]$, **$V_{15}$**, (Fig.1a) are cytotoxic against triple-negative (MDA-MB-231, IC_{50}= 2.53 and 17.2 μM, respectively) and luminal A (MCF7, IC_{50}= 5.68 and 15.1 μM, respectively) breast cancer cell lines.[1] The Wound Healing assay for **V_{10}** (using 0.45 and 0.90 μM) did not show inhibition of cell migration, whereas **V_{15}** (4.3 and 8.6 μM) inhibited migration by 70% and 90%, respectively. SEM images of the MDA-MB-231 cells treated with **V_{15}** (Fig. 1b) revealed a change from fusiform to an epithelial-like morphology, suggesting a reversal of the epithelial-mesenchymal transition, which may be associated with a reduction in tumor aggressiveness.



Conversely for **V_{10}**, it was observed an increase in the number of vesicles, with no major differences in cell morphology. It was already showed that **V_{10}** interacts with G-actin, inhibiting its polymerization with an IC_{50} = 17 μM.[2] Atomic force microscopy (AFM) analysis of actin treated with 40 μM of each POVs evidenced that only **V_{15}** inhibited G-actin polymerization (Fig.1c). These results suggest that **V_{15}** inhibition of G-actin polymerization is associated with the morphological changes in MDA-MB-231 cells, pointing to a possible use as an antitumoral agent against the more aggressive and harder to treat subtype of breast cancer.

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The perferrate puzzle: the challenge of extreme oxidation states in theoretical chemistry

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The search for the highest oxidation states in the first transition metal series has come to the fore in the previous decade. For instance, Li & Schwarz [1] have shown that iron tetroxide $Fe^{VIII}O_4$ is actually metastable and is a precursor of the di-haptic peroxide $[Fe^{VI}O_2(\eta^2\text{-}O_2)]$. Subsequently, the anionic analogues $[FeO_4]^-$ (perferrate) and $[FeO_2(\eta^2\text{-}O_2)]^-$ (peroxoferrate) were detected by Li and Zhou [2] and characterised by mass spectrometry and DFT/CASPT2 calculations. The former can be generated fleetingly by visible light irradiation of the latter, which then decays back into its original form (Figure 1). Unfortunately, the correct stability trend C_{2v}-$[Fe^{V}O_2(\eta^2\text{-}O_2)]^-$ > T_d-$[Fe^{VII}O_4]^-$ was never successfully reproduced by standard computational methods namely CCSD(T), DMRG-NEVPT2/CASPT2 and DFT/B3LYP.

Herein, a re-evaluation of all the hypothetical isomers of perferrate is presented using state-of-the-art multireference configuration interaction (MRCI) approaches to find that an even lower energy isomer exists and that this is the likely species captured by Li and Zhou in their original work [2].

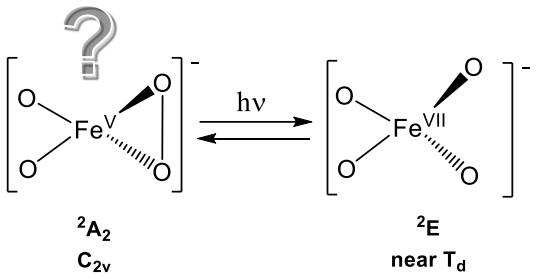

Figure 1. Geometries and computed ground state symmetries of peroxoferrate and perferrate.

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Converting CO_2 with a unique tungsten-dependent enzyme

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Metal-dependent formate dehydrogenases (Fdh) are unique in the catalysis of CO_2 reduction to formate, presenting orders of magnitude higher activities than the metal-independent ones, which are biased for formate oxidation. Formate is a versatile C1 feedstock that can contribute to a carbon-neutral economy.

One of the most active CO_2 reductases described so far is the W/Sec-FdhAB isolated from *Nitratidesulfovibrio vulgaris* Hildenborough. This enzyme has a simple composition and the presence of both W and selenocysteine at the active site contribute to its high CO_2 reduction activity. Enzymes containing W and Sec are usually extremely oxygen sensitive, whereas the W/Sec-FdhAB is surprisingly robust and displays a considerable O_2 tolerance, allowing isolation in aerobic conditions. These properties make it an ideal system for biocatalytic applications towards sustainable CO_2 reduction.

Recently, we showed that the activity of FdhAB is controlled by a redox switch based on an allosteric disulfide bond [1]. The redox switch mechanism operates in vivo and prevents enzyme reduction by physiological formate levels, conferring a fitness advantage during transient cell exposure to O_2.

In order to get further insights into the CO_2 reduction mechanism we constructed several variants of the W/Sec-FdhAB, by mutating the Sec [2] and other conserved residues close to the active site. The variants were characterized in terms of kinetic performance, EPR spectroscopy and structurally by X-ray crystallography. The results provide important insights into the role of first and second coordination residues in catalysis and the overall mechanism, with Sec playing a critical role in the high activity and oxygen tolerance of the enzyme.

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Acknowledgments:

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Green chemistry routes to perovskite nanocrystals for solar cells

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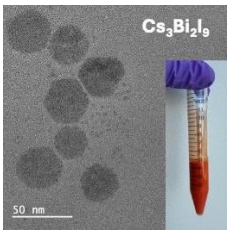
Perovskite nanocrystals have been investigated as quantum materials for the large-scale manufacturing of solar cells.[1] Among the various nanosystems, lead-containing halide perovskites have been studied extensively because they enable high-performance quantum optoelectronic devices. In fact, these quantum structures offer a tunable bandgap, high stability, reduced grain-boundary charge-carriers recombination, narrow emission linewidths, and intense photoluminescence at room temperature. However, conventional chemical approaches for producing such materials also raise toxicity concerns, namely due to the presence of lead ions and the common use of toxic organic solvents during the synthesis. This communication describes our research on greener approaches to perovskite nanocrystals by sequentially exploring sonochemistry methods, vegetable oils as solvents for the synthesis and the use of bismuth, instead of lead, as a less toxic metal in the reduced-dimensional perovskite derivative $Cs_3Bi_2I_9$.[2] Selected examples of solar cells incorporating perovskite nanocrystals synthesised and processed using these greener routes are presented for comparative purposes with common approaches. Although photovoltaic performance validation parameters show that these perovskites are still far from realistic applications, our research clearly demonstrates that greener synthesis routes are viable and are not merely an aspirational goal.



TEM image of $Cs_3Bi_2I_9$ nanocrystals and digital photograph of the respective sample.

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Catalytic strategies for plastic waste upcycling: towards a sustainable circular economy

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Plastics that combine low cost with high performance play a central role in modern society. However, the continuous growth in plastic production, together with the extensive use of plastic packaging, has resulted in serious environmental pollution.

Recycling plastic waste represents an important strategy for achieving sustainability, as it reduces environmental contamination while preserving valuable raw materials. Consequently, significant research efforts have been devoted to developing innovative approaches for recycling plastics or converting them into value-added products. [1]

In continuation of our previous work, this study reports the depolymerization of polyester and polycarbonate plastic waste into a range of valuable and industrially relevant products using environmentally benign homogeneous and heterogeneous catalysts (Figure 1). [2,9]

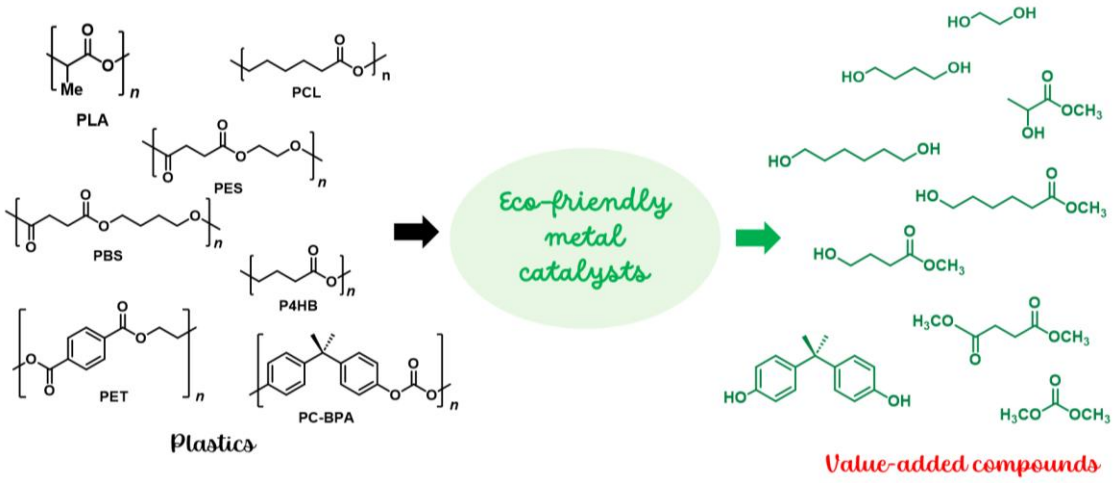

Figure 1. Recycling of plastic waste into value-added compounds using eco-friendly catalysts.

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Metal and carbon-based materials for photocatalytic hydrogen production

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Currently, about 95% of global hydrogen production depends on fossil fuels, resulting in greenhouse gas emissions and low-purity H_2. Developing clean and sustainable alternatives is therefore essential. Photocatalytic water splitting is a promising approach, as it uses abundant solar energy; however, efficient, stable, and low-cost photocatalysts are still needed [1]. In this work, various metal sulfides, metal–organic frameworks, and carbon-based porous materials derived from wastes were synthesized through sustainable approaches (Figure 1). These materials were characterized using several solid-state characterization techniques, such as Powder X-ray Diffraction (PXRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR) spectroscopy, and Diffuse Reflectance Spectroscopy (DRS), and subsequently evaluated as photocatalysts for H_2 production.

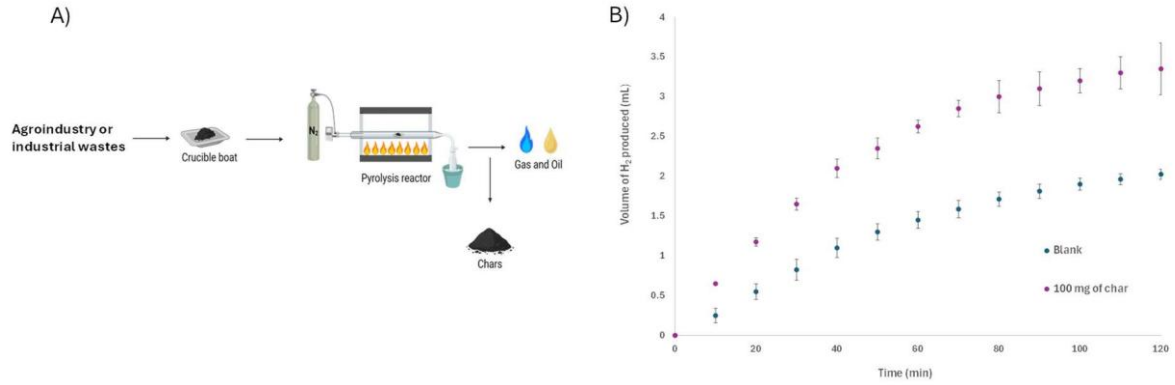

Figure 1: A) Preparation of carbon-based materials from waste residues and B) Photocatalytic H_2 production using a waste-derived carbon material (100 mg) as the photocatalyst and ethanol/water mixture (80:20 v/v) as the sacrificial agent, under irradiation with a 300 W Xe lamp.

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Thermotwin: scalable thermally-chargeable textile supercapacitors based on $MnFe_2O_4$/carbon hybrids

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The rapid expansion of wearable and smart electronics is increasing the demand for lightweight, self-powered textile technologies capable of supplying energy to low-power devices. Thermally-chargeable supercapacitors (TCSCs) have emerged as promising candidates, as they combine thermal energy harvesting with electrochemical energy storage, enabling the direct conversion of body or environmental waste heat into electrical energy.[1,2] However, conventional TCSC architectures typically rely on multilayer assemblies that limit mechanical flexibility and hinder scalability.

In this work, ThermoTwin-TCSCs were developed in a new single-substrate configuration using different electrode materials, including carbon/$MnFe_2O_4$ hybrid (HY) materials, oxidized carbon nanotubes (CNT), graphene (GN), and a CNT/GN mixture. The hybrid nanomaterials were synthesized via an *in situ* coprecipitation route in the presence of the carbon support. The fabrication of the devices involved dual-side coating of the solid-gel electrolyte, followed by screen-printing of the electrode materials. Both symmetric and asymmetric architectures were produced, the latter combining a carbon-based electrode with a hybrid ferrite counterpart. The hybrid asymmetric devices showed markedly higher energy densities than the corresponding symmetric all-carbon counterparts: GN//HY(GN) device exhibited 226% higher energy density than GC//GN (2.03 μWh cm^{-2} *vs.* 0.62 μWh cm^{-2}), and the CNT-GN//HY(CNT-GN) device nearly doubled this output relative to CNT-GN//CNT-GC (3.31 μWh cm^{-2} *vs.* 1.62 μWh cm^{-2}). This enhancement arises from the combination of two energy storage mechanisms: electrostatic charge accumulation at the electrode/electrolyte interfaces (non-faradaic) and faradaic redox reactions from the ferrite. Thermal energy conversion capability was further demonstrated under different real-world thermal gradient scenarios.

These findings underscore the potential of single-substrate TCSCs for lightweight and efficient, energy systems for smart textile applications, paving the way toward self-powered wearables.

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Development of manganese porphyrins as redox-sensitive MRI contrast agents

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The design of MRI contrast agents (CAs) capable of sensing changes in the cellular microenvironment represents a promising strategy for early disease diagnosis. In particular, alterations in tissue redox status serve as important biomarkers for a variety of pathologies. In light of recent safety concerns surrounding Gd^{3+}-based MRI agents and the need for more biocompatible alternatives, we are developing novel probes based on manganese (III) tetrapyrrolic macrocycles. [1–3] They attractive in this context because they can stabilize manganese in both the high-spin, paramagnetic Mn(II) and Mn(III) oxidation states, providing an ideal platform for redox-responsive MRI probe design.

Herein, we report the synthesis of a series of porphyrins and their complexation with manganese. UV–Vis spectroscopy and $^{1}H/^{19}F$ NMR measurements demonstrate that these complexes undergo reversible Mn(III)/Mn(II) reduction in the presence of a biological reductant such as ascorbic acid, with reoxidation occurring upon exposure to O_2. ^{1}H nuclear magnetic relaxation dispersion (NMRD) profiles were obtained for both oxidation states. The Mn(III) complexes exhibit higher ^{1}H relaxivities at elevated magnetic fields, whereas the Mn(II) analogues show enhanced relaxation efficacy at low magnetic fields. Importantly, the redox transformation can be visualized in both ^{19}F and ^{1}H MRI phantom images at 7 T.

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Rapid microwave-assisted synthesis of benchmark Iron(II) complexes

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Organometallic complexes are central to modern chemistry, with applications in catalysis, functional materials, and biomedicine. Among them, monocyclopentadienyliron(II) compounds have emerged as promising anticancer candidates [1,2], with tuneable electronic and structural properties through ligand design, enabling development of new therapeutic and imaging agents. While these complexes can be prepared via conventional or non-traditional methods, such as microwave irradiation, developing alternative routes is key to accelerating progress towards more advanced drug candidates - replacing hazardous solvents, improving yields, and shortening reaction times.

This work explores microwave-assisted synthesis (MAS) as an efficient route to octahedral complexes $[Fe(L\text{-}L)_2(L')_2]^{2+}$ and $[Fe(L\text{-}L)_3]^{2+}$ (L-L = N,N-bidentate ligands), and monocyclopentadienyliron(II) derivatives $[Fe(\eta^5\text{-}C_5H_4R)(L\text{-}L)(L')]^+$ (R = H, $COCH_3$; L-L = N,N- or P,P-bidentate; L' = CO, PR_3, I, etc.) (Figure 1). Compared with conventional heating, MAS offers rapid, homogeneous heating, markedly shorter reaction times, improved yields, and reduced environmental footprint [3]. We optimised synthetic routes and key intermediate steps to maximise efficiency, including solvent replacement with greener options, providing more sustainable and practical access to these iron(II) complexes.

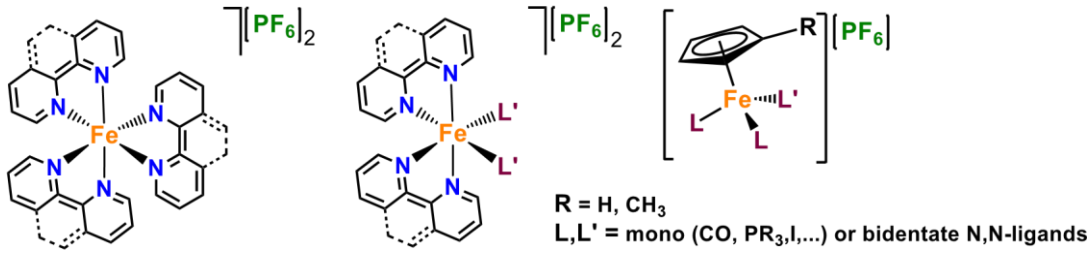

Figure 1 – General structures of the synthesised complexes

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Metal-induced biofilm formation in *Deinococcus radiodurans*

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A biofilm is defined as a community of microorganisms embedded in a self-produced polymeric matrix composed of extracellular polymeric substances secreted by the bacteria. Biofilms are highly relevant in multiple fields, including clinical and biotechnological applications. However, biofilm formation and its potential applications, in radiation-resistant bacterial strains such as *Deinococcus radiodurans* and *Deinococcus indicus*, have not been thoroughly explored. In this study, we tested various conditions to induce biofilm formation in both *Deinococcus* strains and investigated their potential use in the bioremediation of toxic metals, namely for the detoxification of arsenate. Using Scanning Electron Microscopy, we demonstrated that manganese or iron promotes biofilm formation, providing the first evidence of biofilm formation in *D.radiodurans* and showing that metals play a crucial role in this process.

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FGFR-Targeted ruthenium–peptide conjugates with pH-responsive linkers for selective breast cancer therapy

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Metastatic breast cancer (MBC) remains a major clinical challenge, accounting for a substantial proportion of breast cancer diagnoses and still lacking curative treatment. Although therapeutic options have expanded, their efficacy remains limited and is frequently associated with severe side effects due to poor selectivity [1]. To address this unmet need, we are developing smart metallodrug delivery systems (SMDS) based on ruthenium complexes, designed to target both primary tumors and metastatic [2]. Our strategy incorporates a peptide with high affinity for fibroblast growth factor receptor (FGFR), which is overexpressed in approximately 20% of breast cancers, thereby promoting selective accumulation. This peptide is covalently linked to a cytotoxic Ru(II)(η^5-C_5H_5) complex through a linker designed to undergo cleavage under the mildly acidic conditions of the tumor microenvironment, enabling controlled activation of the metal complex only at the tumor site. In this work, we explore different pH-sensitive linkers to conjugate Ru complexes to FGFR-selective peptides, using either the cyclopentadienyl or bipyridine ligands as conjugation sites. The synthesis and characterization of these Ru–peptide conjugates, together with their drug-release profiles under pH conditions that mimic both the bloodstream and the tumor microenvironment, will be presented. The three-dimensional conformational structures of the free peptide and the conjugate were elucidated by NMR spectroscopy. The cytotoxic activity of these systems was evaluated in four breast cancer cell lines with varying FGFR expression levels, under pH conditions that mimic both the tumor microenvironment and the bloodstream. Furthermore, the interactions of the free peptide, the Ru(η^5-C_5H_5) complex, and the lead Ru–peptide conjugate with human serum albumin will be investigated to gain insight into their potential blood transport mechanisms.

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Poster Communications

Efficacy of redox−active Cu(II) dipyrrin complexes toward electrochemical reduction of CO_2

P1

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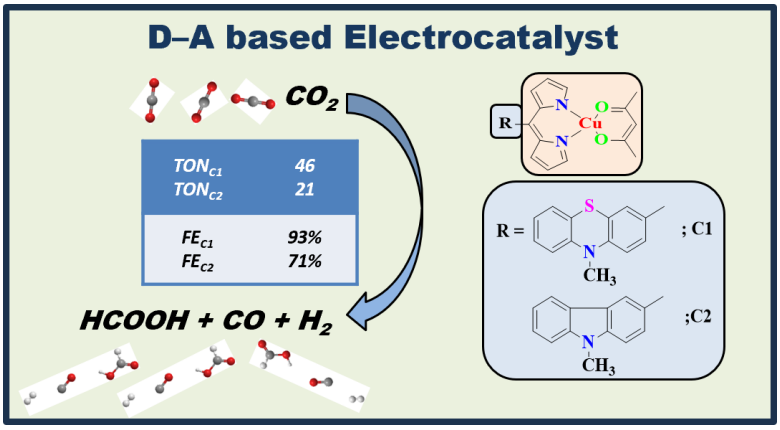

New D−A-type catalysts based on Cu (II) complexes (**C1** and **C2**) including dipyrrin ligands with phenothiazine/carbazole as the meso-substituent have been described. The complexes have been thoroughly characterized by various methods (^{1}H, ^{13}C, ESI−MS, EPR, and UV−vis studies), and structures of both **C1** and **C2** unequivocally determined by Xray single crystal analyses. The catalysts **C1** and **C2** are stable at room temperature and exhibit Faradaic efficiency values of ~56% (**C1**) and ~ 46% (**C2**) toward homogeneous reduction of CO_2 to CO. The release of CO has been validated by gas chromatographic (GC) studies. Electron-rich phenothiazine and carbazole included in the catalysts facilitate proton transfer, enabling rapid and selective formation of CO over H_2 with FE_{H2} values of ~22% for **C1** and ~7% for **C2** and turnover numbers (TON) of ~46 for **C1** and ~21 for **C2**. Furthermore, the formation of formate ions has been affirmed by ion chromatography (**C1**, ~16%; **C2**, ~18%). Detailed electrochemical studies and product analyses suggested that **C1** displays superior catalytic activity relative to **C2** which has been further supported by theoretical studies.

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Unveiling the unusual function of 4-helix bundle proteins from anammox bacterium *brocadia pituitae*

P2

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Anammox (Anaerobic Ammonium Oxidizing) bacteria have high iron requirements, since their genome encodes for an abundant number of iron-containing proteins that are involved in their growth and metabolism. These enzymes participate in the anaerobic oxidation of NH_4^+ to N_2, with nitric oxide as an intermediate, resulting in a more efficient process for removing ammonia from wastewater treatment plants than the nitrification-denitrification process[1, 2]. However, when iron is present in high amounts, it can trigger accumulation of toxic intermediates, such as reactive oxygen species and Fe^{3+}, and consequently the destruction of cellular components[1]. Thus, microorganism developed mechanism to allow iron sufficiency and simultaneously prevent iron-induced and oxidative stress toxicity, namely four-helix bundle proteins such as hemerythrins, rubrerythrins and the ferritin-like super family, all involved in iron metabolism and regulation of oxidative stress. In these work, the biochemical and biological characterization of unusual four-helix bundle proteins, such as two one-domain rubrerythrins and one bacterioferritin, from the Anammox organism *Candidatus Brocadia pituitae* will be discussed. Sequence analysis and structure prediction will be presented as well as iron loading ability and substrate determination which were studied by UV-Visible spectroscopy. Their DNA binding ability was assessed by electrophoretic techniques and fluorescence confocal microscopy assays. One-domain rubrerythrins can use both O_2 and H_2O_2 as substrates for the ferroxidase reaction, and are capable of oxidizing 100 Fe^{2+}/dimer, while bacterioferritin also use O_2 and H_2O_2 as substrates, but can oxidize 4000 Fe^{2+}/24-mer. All proteins in this study were able to bind DNA in the absence of iron and trigger DNA condensation, but when iron was added, these proteins lost this ability. The DNA binding and aggregation ability dependent on the presence or absence of iron combined with the capacity to use both O_2 and H_2O_2 as substrates for the ferroxidase reaction suggests a new mechanism of DNA protection in bacteria.

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Surface modification of Iron oxide with glycine Imines for hyperthermia Applications

P3

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Magnetic Hyperthermia Therapy (MHT) has emerged as an alternative cancer treatment, utilizing magnetic nanoparticles to generate localized heat (42–45°C) under an alternating magnetic field to selectively induce apoptosis in cancer cells. Due to their biocompatibility and robust magnetic properties, iron oxide nanoparticles (Fe_3O_4) are ideal candidates for this application, as their surfaces can be easily modified to enhance functionality.

This study focused on the synthesis and characterization of Schiff base-functionalized Fe_3O_4 nanoparticles, modified via glycine and aldehyde attachment, to evaluate how these coatings influence magnetic behaviour. All tested samples exhibited superparamagnetic behaviour at room temperature. In the magnetization curves, the saturation of the NPs decreased from about 70 emu/g for Fe_3O_4 to a range between 18 and 30 emu/g. The decrease in saturation curves resulted from the surface coating and surface functionalization of Fe_3O_4 nanoparticles. Among the synthesized MNPs, Fe_3O_4@(2-hydroxybenzylidene(ethyl)amine) (MNP 3) showed a higher saturation magnetization. Magnetic Hyperthermia measurements revealed heat production in all NPs; however, SAR values decreased when Fe_3O_4 was coated on the surface.

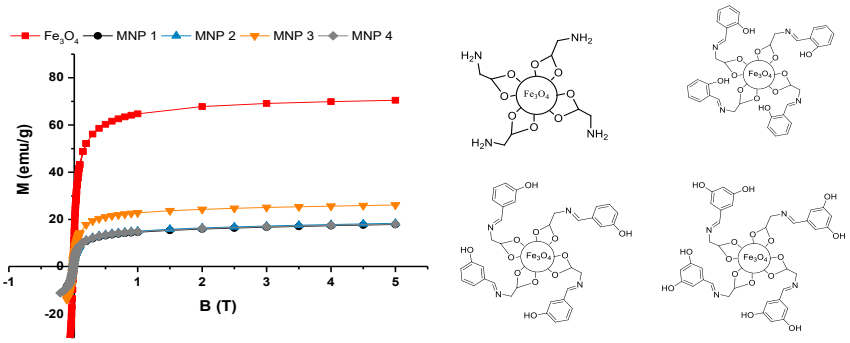

Figure 1: Magnetic saturation curves of samples at 300 K.

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Bis(oxinate)polyamines as chelating ligands for theranostic applications

P4

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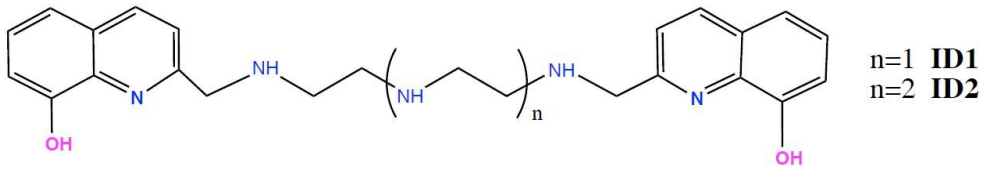
In 2022, cancer caused the death of around 10 million people and almost 20 million new cases were detected worldwide, according to WHO [1]. Early diagnosis and prompt treatment are appointed as main strategies to reduce cancer mortality by one third [2]. In this context, molecular nuclear imaging has emerged as a valuable diagnostic tool and a rapidly growing research field [3]. Tumor detection is achieved by tracing particles emitted by the decay of radionuclides, often radiometals, that minimally interact with body tissues [3]. Typically, radiometals are bound to a chelator that prevents metal ion's toxicity in biological media [3]. Consequently, new chelators are continuously being synthesized to achieve more adequate binding to radiometals. 8-Hydroxyquinoline (8HQ, oxine), a quinoline derivative, is a relevant scaffold in medicinal chemistry due to its pharmacological effects and provides good chelating moieties for metal coordination [4]. 8HQ containing chelators have proved to be good chelators for metal ions such as Cu(II) and Ga(III), with an easy and straightforward synthesis [5] [6]. However, they are insoluble in aqueous media and buffer systems [5]. To overcome this drawback, new chelators (ID1 and ID2) have been synthesized to better accommodate these metal ions. Their properties and stability in biological media is studied both experimentally and computationally.



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The synthesis of innovative curcumin based metal complexes for the development of luminescent materials with potential anticancer activities

P5

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Curcumin, an orange-yellow natural polyphenol extracted from the rhizome of Curcuma longa (turmeric), is widely known as a culinary spice in Asian countries and as a key component in traditional Chinese and Indian medicine due to its many beneficial properties, including anti-inflammatory, antimicrobial, antioxidant and anticancer effects. Although curcumin has shown numerous beneficial effects on human health, several shortcomings hinder its therapeutic potential. The most important drawbacks are its low aqueous solubility, its chemical instability, and rapid metabolic degradation, all contributing to curcumin's poor bioavailability, while curcumin is also recognized as a panassay interference compound (PAINS). In this research it is attempted to increase both the bioavailability and anticancer potential of curcumin by simultaneously modifying its chemical structure, while also coordinating these biomolecules with various metal ions. Thus, a library of curcuminoid rare earth complexes was synthesized by combining curcumin and some new derivatives (with 3-pyridyl, 2-pyridyl, 4-methylbenzyl and 3-thienyl ring structures) with different rare earth metals (europium, lanthanum, lutetium, neodymium, gadolinium and yttrium). FT-IR and ^{1}H NMR spectroscopy revealed that in the case of yttrium and lutetium complexation, one metal complex is formed selectively for curcumin and all selected derivatives. When lanthanum is deployed to coordinate to the curcuminoids, a more complicated behavior is noticed, presumably resulting in a mixture of different complexes. For the 3-pyridyl curcuminoid, however, it seems possible to force the coordination with lanthanum toward only one type of complex when adding an excess of the base triethylamine. In the near future, additional structural characterization and biological testing of the resulting complexes will be pursued.

Cellulose-derived materials loaded with coordination polymers for antimicrobial applications

P6

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Antimicrobial resistance (AMR) is an emerging global health issue associated with the spread of bacteria and the formation of biofilms [1]. In this context, biobased polymers derived from polysaccharides and combined with bioactive coordination polymers (bioCPs) can offer biodegradability, biocompatibility, and controlled release of antimicrobial agents. These properties make them a promising strategy for preventing bacterial growth and accumulation, inhibiting biofilm formation, and reducing cross-contamination [2,3].

This work presents the synthesis and full characterization of two new Ag(I) bioCPs, $[Ag(msba)]_n$ (**CP1**) and $[Ag(Ksba)(H_2O)_2{\cdot}2H_2O]_n$ (**CP2**), self-assembled from a silver(I) salt and a benzoic acid-based building block, namely 4-(methylsulfonyl)benzoic acid (Hmsba) and 4-sulfobenzoic acid monopotassium salt (KHsba). These compounds were used as antimicrobial doping agents in cellulose acetate and ethylcellulose films to produce hybrid materials.

The bioCPs and hybrid biopolymer films were evaluated for their antibacterial and biofilm inhibition activities against Gram-positive (*S. epidermidis* and *S. aureus*) and Gram-negative (*P. aeruginosa* and *E. coli)* bacteria and respective biofilms. The materials demonstrated promising antibacterial and biofilm inhibition activity, highlighting their potential as antimicrobial coating materials for applications in healthcare, packaging, and high-touch surfaces.

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Acknowledgments: This work was financially supported by the FCT (PolyBioPrint 2023.14308.PEX, 2022.09436.BD, UID/00100/2025, UID/PRR/00100/2025, LA/P/0056/2020, CEECIND/02725/2018, CEECIND/00194/2020), the IPL (IPL/IDI&CA2024/Gel2Heal_ISEL project), and the MINDlab (https://MINDlab.pt).

Recent developments in topical photodynamic therapy using reduced porphyrin as photosensitizer

P7

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Photodynamic therapy (PDT) uses a photosensitizer, light, and oxygen to produce reactive oxygen species (ROS) that cause oxidative stress and cell death.[1] It is commonly used to treat skin conditions such as basal cell carcinoma and squamous cell carcinoma.[2] However, its effectiveness in melanoma is limited due to factors like strong antioxidant defenses, defective apoptotic pathways, neoangiogenesis, and melanin interference.[3] In this communication, we report the purification, the revalidation of the photochemical properties (ε_{733} = 1.0x10^5 M^{-1} cm^{-1}, Φ_F= 0.16, Φ_{pd}= 1.5x10^{-4}, Φ_Δ= 0.39), and comprehensive rheological characterization of a thermosensitive gel formulation resulting in different gelation temperatures.[4] The therapeutic potential was evaluated by a comparison between IV administration, which achieved cured mice in one treatment, and passive/active permeation by topical application.[4]

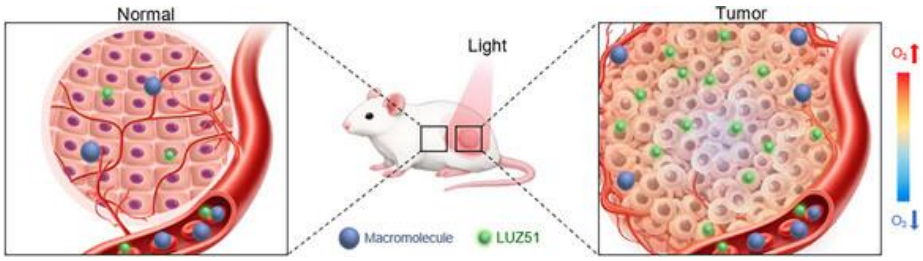

Figure 1: Schematic PDT treatment

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Acknowledgments:

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Group 6 bis-triazolylidenes in metal-ligand cooperative dehydrogenation of alcohols

P8

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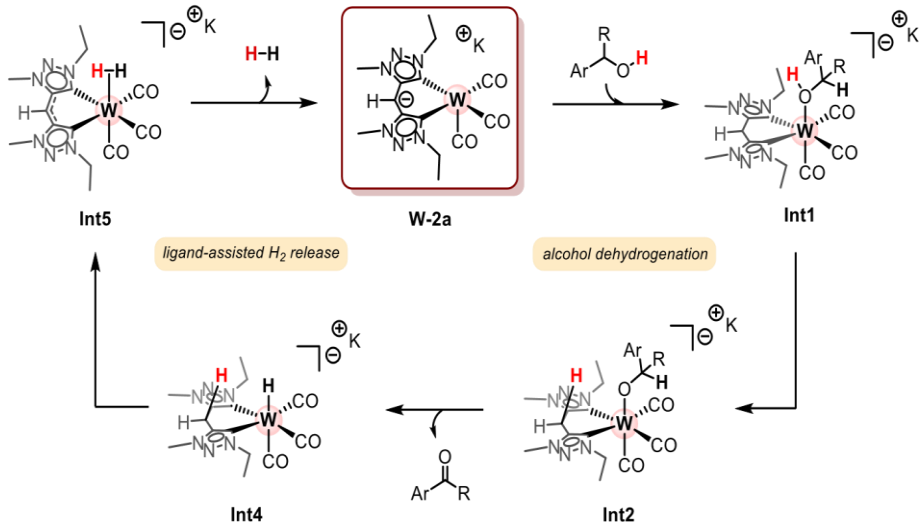
Acceptorless dehydrogenative coupling (ADC) represents a sustainable approach for C–C and C–N bond formation, enabling the synthesis of *N*-heterocycles from alcohols, with H_2 and H_2O as the only by-products. Despite their earth abundance and rich redox chemistry, group 6 metal complexes (Cr, Mo, W) remain largely underexplored in ADC catalysis, particularly in combination with *N*-heterocyclic carbenes and mesoionic ligands. Herein, we report a new family of Cr, Mo, and W tetracarbonyl complexes supported by a methylene-bridged bistriazolylidene ligand and evaluate their catalytic activity in quinoline synthesis via ADC.[1] All complexes are catalytically competent, with the tungsten derivative showing superior performance. Experimental and DFT studies revealed an unprecedented base-induced deprotonation of the methylene bridge, generating a methylidene intermediate that enables metal-ligand cooperativity. The deprotonated bridge acts as an internal base during alcohol activation and participates in the H_2 release, providing the first evidence of cooperative reactivity in these systems operating in ADC.



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Acknowledgments:
We thank FCT for projects 2023.17853.ICDT, 10.54499/PTDC/QUI-QIN/0359/2021, MOSTMICROITQB R&D Unit, LS4FUTURE (LA/P/0087/2020), CERMAX, Campus Iberus and EU's Horizon 2020Marie Skłodowska program (No. 101034288). B. G. thanks FCT for PhD grant 2024.01254.BD.

Sustainable copper(i)–NHC catalysts for the efficient synthesis of imines and propargylamines

P9

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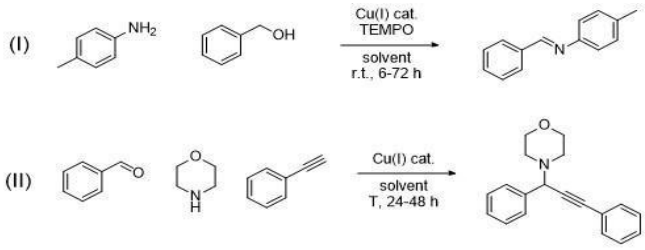
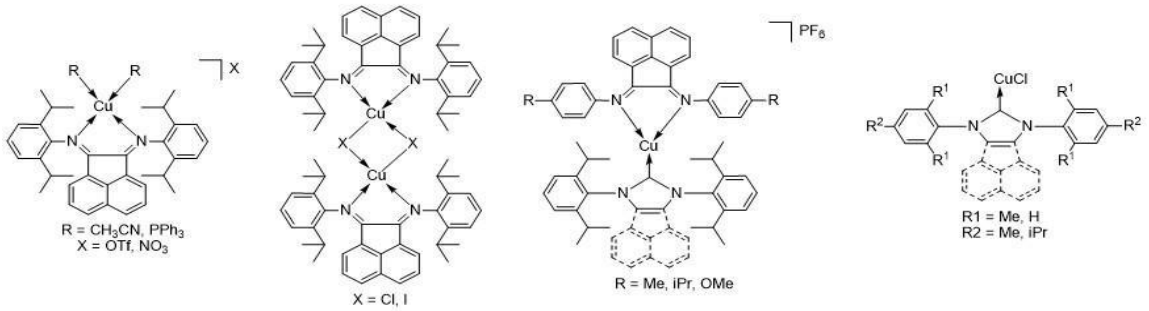
The development of sustainable catalytic methodologies remains a central goal in modern synthetic chemistry, particularly for the preparation of pharmaceutically relevant compounds. In this study, a series of copper(I) complexes were synthesised and evaluated as catalysts for two related transformations: the formation of imines via the aerobic oxidation of alcohols with amines [1], and the A³ coupling of aldehydes, amines and alkynes to produce propargylamines [2], derivatives which are valuable intermediates in pharmaceutical chemistry. Particular emphasis was given to heteroleptic copper(I) complexes containing bis(imino)acenaphthene (BIAN) and *N*-heterocyclic carbene (NHC) ligands. The combination of these ligands provides electronic tunability and stability to the copper centre. Copper was selected due to its low cost and low toxicity. The synergistic combination of these ligand frameworks around the copper center was explored to enhance catalytic efficiency and selectivity.

The catalytic activity of the synthesised complexes was evaluated in both reactions, demonstrating the potential of Cu(I)BIAN-NHC systems as effective and sustainable catalysts for synthesising nitrogen-containing compounds.



Cu(I) catalysts synthesized in this work for the catalytic formation of imines and propargylamines:



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Acknowledgments:
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Turning the light on cadmium at physiological pH

P10

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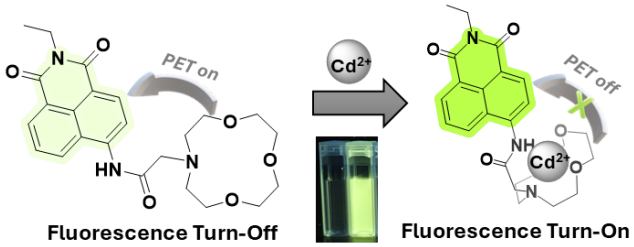

Cadmium (Cd) is a toxic heavy metal with no biological role know, and its accumulation in the environment, caused by anthropogenic activities such as industrial processes, waste management, fossil fuel combustion, and phosphate-based fertilizers, results in a significant ecological and health risks. Human exposure occurs primarily through contaminated food and water, with cadmium's high affinity for biological tissues — particularly the kidneys — leading to bioaccumulation and prolonged retention. Chronic exposure has been linked to renal dysfunction, osteoporosis, cardiovascular diseases, and systemic health issues, underscoring the urgent need for effective detection methods.[1] Fluorescent chemosensors have emerged as an effective solution for detecting and precisely quantifying metal ions, particularly as conventional methods like Atomic Absorption Spectroscopy (AAS) and Inductively Coupled Plasma Optical Emission Spectrometry (ICP-AES) are expensive and involve intricate sample processing.[2, 3] These chemosensors can provide a unique response in the presence of target analytes, even at trace levels, making them a more economical and efficient alternative.[4] In this context, azacrown derivatives are well known for their ability to interact with various metal ions. In this work, a naphthalimide was functionalized with an azacrown moiety to serve as potential fluorescent chemosensors for metal ions. To investigate the photophysical characteristics of these compounds, UV-Vis and fluorescence titrations were carried out with a range of metal ions. The results of these experiments demonstrated a selectivity towards cadmium (K= 1.53×104 M^{-1}) and a LOD value of 73.6 nM.

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Design, synthesis and characterization of PMC79 derivatives for KRAS-mutated cancers

P11

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KRAS mutations are present in 90% of pancreatic cancers [1], as well as in about 45% of all colorectal cancers and 35% of all non-small-cell lung cancers [2]. Although various studies have attempted to create a drug that targets these mutations, KRAS mutations are still labelled as undruggable.

In the last few years, a new compound, PMC79 – [Ru(□^{5}-C_5H_5)(2,2'-bipyridine-4,4'bis(hydroxymethyl))(PPh_3)][CF_3SO_3], has been found to target three of KRAS most common mutations, namely G12V, G12D and G13D [3]. With this project, we aim to optimize PMC79's structure to enhance the efficacy, selectivity, and pharmacokinetic properties by developing a backup library which will also strengthen R-nuucell's intellectual property portfolio. We synthetised the PMC79 cation bearing different counter-anions, first through conventional organometallic synthesis methods and then via microwave-assisted reactions. The new compounds were then characterized using solubility and stability studies in physiologically relevant conditions. A comparative analysis of the two methodologies was performed on experimentally relevant parameters, providing a comprehensive basis for evaluating the strengths and limitations of conventional versus microwave-assisted methodologies in the synthesis of the PMC79 cation.

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Acknowledgements: Fundação para a Ciência e Tecnologia is acknowledged for Projects/Grants UID/00100/2025 (DOI: 10.54499/UID/00100/2025; CQE), UID/04046/2025 (DOI: 10.54499/UID/04046/2025; BioISI), 2023.10475.CPCA (DOI: 10.54499/2023.10475.CPCA.A2; PJC), 2025.00994.BDANA (AFG), 2023.15441.TENURE.002/CP00003/CT00014 (AV), and 2023.15441.TENURE.008/CP00003/CT00005 (PJC).

New copper and silver complexes as antimicrobial dopants for 3d printed biopolymer materials

P12

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In pursuit of our research on antimicrobial materials [1-4], this work reports the synthesis, characterization, and properties of a novel series of hybrid biopolymer composites containing bioactive metal complexes. Four new Cu and Ag coordination compounds were synthesized using *t*-butyl tosyl carbamate (HTBT) and *p*-toluene sulfonyl urea (HPTSU) as building blocks. These ligands were selected because of their proven ability to enhance antimicrobial activity and bypass bacterial resistance mechanisms when coordinated to metal centers. The obtained compounds were characterized by standard methods, including by single-crystal X-ray diffraction, and formulated as $[Cu(TBT)_2(H_2O)_2]$, $[Ag(TBT)(NH_3)]$, $[Cu(PTSU)_2(H_2O)_2]$, and $[Ag(TBT)(NH_3)]$. Both Cu and Ag complexes were integrated as bioactive dopants into corn starch (CS) formulations to produce antimicrobial biopolymer composites.

For printing of 3D biopolymer materials, the methodology consisted of using the 3D syringe extrusion printing technique, based on G-code and digital CAD models for varying complexity, which were subsequently rendered and adjusted with optimized printing parameters. The CS/glycerol/dopant blends were calibrated for precise extrusion and structural stability. The resulting biopolymer films where characterized by SEM, TGA, and mechanical tests (tensile strength and elongation properties). The incorporation of coordination compounds into degradable biopolymer matrices opens up new possibilities for the production of active packaging materials capable of inhibiting microorganism growth.

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Acknowledgments:

This work was supported by FCT (PolyBioPrint-2023.14308.PEX, UID/00100/2025, UID/PRR/00100/2025), IPL/IDI&CA2024/Gel2Heal_ISEL project, CAPES (CNPq/DAI #140275/2024-0, and CAPES/PDSE #88881.127085/2025-01) and MINDlab (https://MINDlab.pt).

Effects of metalation on watson-crick base-pairing of metalated guanosine

P13

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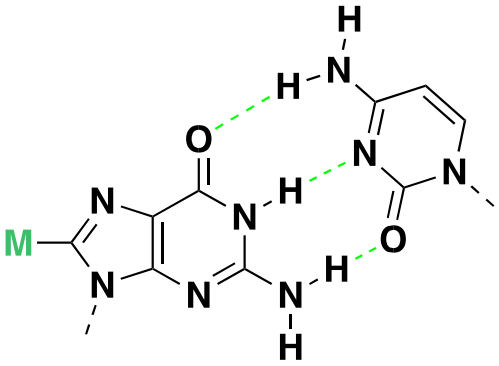
Base pairing is fundamental to nucleic acid structure and function, ensuring accurate DNA replication and transcription through specific hydrogen-bond interactions between complementary nucleobases. In RNA, Base pairing is essential for forming secondary and tertiary structures—such as stem-loops and hairpins—that govern RNA stability, regulate gene expression, and enable functions in processes like translation or splicing, among others.



In our research group we explore the modification of nucleosides with metal complexes and study their subsequent reactivity: Specifically, for metalated nucleobases where all the sites involved in base-pairing are intact, we study how the introduction of a metal affects the signature properties of the nucleobase regarding base pairing. We have synthesized the metalated guanosine derivatives and examined by ^{1}H NMR the ability of the organometallic nucleoside to undergo Watson-Crick base pairing. The results of this work will be discussed in this communication.

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Improving the photodynamic activity of metallochlorins by combined computational design and experimental validation

P14

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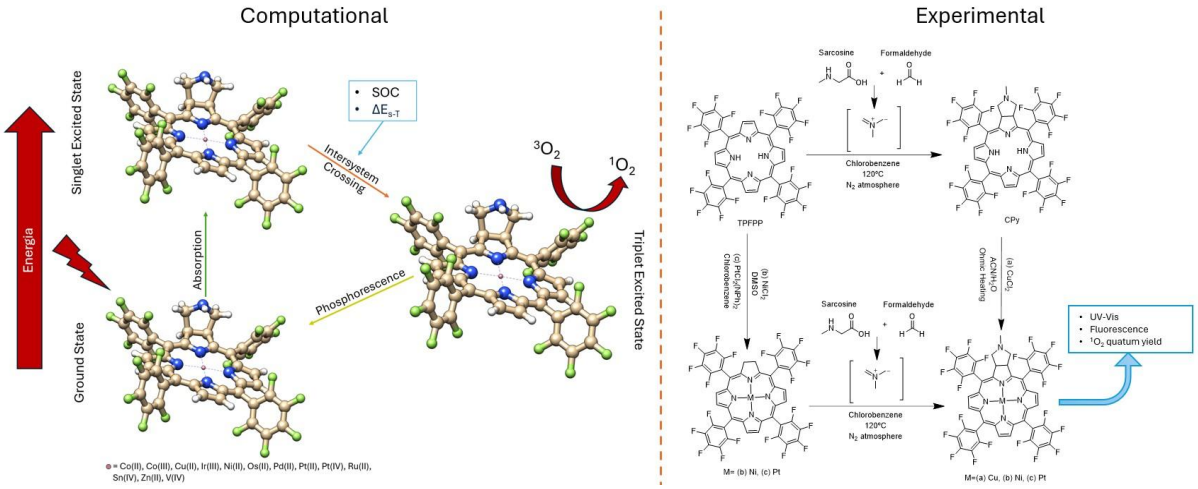
Photodynamic therapy (PDT) employs light-activated photosensitizers (PS) to generate reactive oxygen species for cancer treatment,[1, 2] with efficiency strongly influenced by their photophysical properties, which can be modulated through structural modifications, such as metal coordination.[3] Using DFT and TDDFT-TDA calculations and Spin–orbit coupling (SOC) values, we investigated how different metal centers affect chlorin derivatives, showing that heavy metals, particularly Pt, markedly increase SOC and favor singlet oxygen generation, whereas complexes with low T_1 energy gaps (<0.98 eV) are predicted to be inactive. Pt-, Ni-, and Cu-chlorin complexes were synthesized, and singlet oxygen measurements using DPBF under LED irradiation confirmed the trends: PtCPy showed high activity, while NiCPy and CuCPy were inactive.



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Exploring the solubility and metal binding ability of 8-hydroxyquinoline derived molecules

P15

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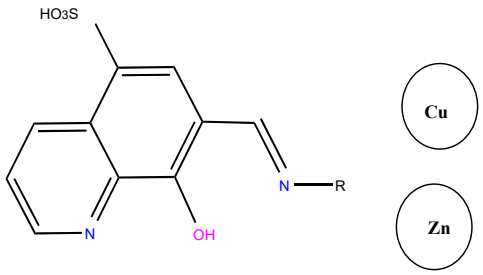
Cancer is one of the most devastating diseases causing approximately 9,7 million of deaths in 2022 according to GLOBOCAN [1]. Metal complexes, using trace metals like Zn, and Cu, can exhibit redox potential (Cu) and a vast array of geometries and coordination numbers, showcasing their potential as anticancer agents [2]. 8-hydroxyquinoline (O,N donor) is a privileged structure and can be functionalized to tune biological properties including anticancer activity, however it displays poor aqueous solubility [3]. Schiff bases are structural moieties with ability to bind to DNA and induce apoptosis, usually displaying potent anticancer activity as well [4]. In order to improve the aqueous solubility of 8-hydroxyquinoline, functionalization at position 5 with a sulfonic acid (SO_3H), and at position 7 with imine donors, was performed aiming to enhance solubility and stability, and to create novel drug-candidates with anticancer activity.

Several ligands and metal complexes were synthesized and characterized in solid state and solution by analytical and spectroscopic techniques. Their stability in organic and buffered media was evaluated, as well as their emissive properties.



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Novel ruthenium complexes containing (iso)nicotinic acid ligands: synthesis and cytotoxic activity

P16

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Cancer remains one of the deadliest diseases in the world, with more than 10 million cancer-related deaths reported in 2022. Due to the insufficient efficacy and severe side effects of current cancer treatments, research has been focused on developing alternative therapeutic methods [1].

Among these, ruthenium complexes have become highly promising candidates for cancer therapy, namely organometallic half-sandwich ruthenium(II)–arene complexes. Our group has been focused on developing complexes with the Ru(η^5-C_5H_5) (RuCp) moiety, having obtained encouraging results in terms of anticancer and antimetastatic properties, both in vitro and in vivo. The complex with the structure [RuCp(PPh_3)(bipy)][CF_3SO_3] (TM34) is the most promising to date, having shown higher cytotoxicity than cisplatin in several cancer cell lines (breast, ovarian, prostate, leukemia and more), and its effect was discovered to be linked to its distinct therapeutic target, the cell membrane [2].

Aiming at modulating the biological properties of TM34, we decided to synthesize two new RuCp(II) complexes by incorporating two bioactive ligands on the Cp ring, namely nicotinic acid (vitamin B3) and isoniazid, which have garnered recent attention in cancer research [3]. Herein, we report the synthesis and full characterization of the two complexes with the general formula [Ru(η^5-$C_5H_4CCH_3$=R)(PPh_3)(bipy)][CF_3SO_3], where R = NNHCO(py-3-yl) (nicotinic acid derivative) or NNHCO(py-4-yl) (isoniazid derivative). After spectroscopic characterization, we detected the presence of E/Z-hydrazone isomerism, which was confirmed by density functional theory calculations. The stability of the complexes in biological media was evaluated, and their cytotoxicity was determined in vitro in a panel of cancer cell lines: human melanoma (A375), human alveolar adenocarcinoma (A549), human epidermoid carcinoma (A431), and human breast cancer (MDA-MB 231).

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Cyclopalladated complexes with functionalized diphosphanes as promising antifungal scaffolds

P17

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Invasive candidiasis, caused by Candida species, is associated with high mortality and morbidity in hospital settings.[1] While Candida albicans remains the most prevalent pathogen, non-albicans species such as Candida parapsilosis and the emerging, pan-resistant Candida auris present significant clinical challenges.[1] These factors, combined with the scarcity of effective antifungals, have led the World Health Organization to prioritize several Candida species for urgent research and drug development.[2]

Because of this scenario, a more diverse library of antifungal drugs is urgently needed, as all approved drugs so far are organic molecules.[3] Palladium complexes have attracted considerable attention due to promising biomedical applications, showing remarkable anticancer and antibacterial activity.[4] However, their antifungal potential remains largely unexplored.[3]

Here, we report the synthesis, characterization, and antifungal activity of new cyclopalladated complexes against several Candida species. Our findings highlight the potential of palladium-based scaffolds as a new avenue for antifungal drug discovery.

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Crfevw*x* (x = Ta or Ti) high-entropy alloy: a theoretical and experimental comparative investigation on phase stability

P18

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Materials capable of withstanding extreme environments are the best candidates for nuclear fusion reactors. In this study, equiatomic CrFeVW*X* (*X* = Ta or Ti) high-entropy alloys (HEAs) are studied as interlayer materials between W and CuCrZr. Monte Carlo (MC) and Molecular Dynamics (MD) simulations predicted a bcc-type structure for both systems, with a lower potential energy and a more stable structure for both systems predicted by MC. For CrFeTaVW, the chemical segregation values are lower in MC than in the MD, whereas for CrFeTiVW, the opposite trend is observed, with MC indicating stronger segregation values. After simulation, the HEAs were prepared by planetary ball milling, consolidated by spark plasma sintering, and analyzed using X-ray diffraction, scanning electron microscopy, and thermal diffusivity. The experimental results for the milled powders confirmed the formation of a bcc structure in both alloys. The consolidated materials presented a bcc-type structure and an Fe_2Ta Laves phase for the CrFeTaVW, while the CrFeTiVW exhibits two different bcc-type structures. The values of CrFeTaVW and CrFeTiVW thermal diffusivity are between 3.5 and 7mm2/s, which is consistent with the expected values for HEAs. Overall, the findings indicate that these HEAs have promising properties that can be used in extreme environments.

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Photocatalytic performance of SnO_2 nanoparticles: when doping is not enough

P19

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SnO_2 is a promising photocatalyst due to its robustness, low cost, and environmental compatibility; however, its wide band gap severely limits its efficiency under visible light. In this work, Mn- and Co-doped SnO_2 nanoparticles, including co-doped systems, were produced to overcome this limitation and to enhance photocatalytic performance toward the degradation of emerging pollutants.

Pristine and Mn, Co (co-)doping SnO_2 nanoparticles were successful produced by hydrothermal treatment of an amorphous single-precursor[1]. The doping with Mn and Co successfully modified the optical properties of pristine SnO_2 nanoparticles, as evidenced by diffuse reflectance measurements. In addition, X-ray powder diffraction confirmed the preservation of the SnO_2 crystalline structure upon incorporation of Mn and/or Co. Photocatalytic degradation experiments were carried out using caffeine and Rhodamine B as model pollutants. Despite these promising optical features, mainly the improvements on the absorption band edge, the photocatalytic performance of doped nanomaterials remained limited. These results clearly demonstrate that band gap engineering through metal doping, although widely pursued, is not always the best methodology to enhance the photocatalytic potential of metal oxides nanoparticles, like SnO_2. Thus, this work underscores a critical limitation of (metal) doping strategies and highlights the urgent need for alternative approaches—such as heterostructure design or defect engineering—to achieve meaningful advances in photo-assisted catalytic processes, including in effective photocatalytic materials for environmental applications.

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Biochemical characterization of nitrous oxide reductase from Stutzerimonas Stutzeri

P20

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N_2O release to the atmosphere has risen 20% from pre-industrial levels and it is now jeopardizing the climate goals of the Paris Agreement. The increase in the N_2O release is mainly due to anthropogenic activities associated with the food industry and the use of fertilizers in agriculture. Nitrous oxide, being a potent greenhouse and ozone depleting molecule, has also indirect health problems, such as an increased risk of skin cancer due to the increased exposure to ultraviolet radiation, and climate change can contribute to respiratory problems and spread of infectious diseases.

The enzyme nitrous oxide reductase (N_2OR) is the only enzyme in Nature known to efficiently reduce N_2O to N_2, an inert gas [1]. In here, we present the optimization of the purification procedure of the recombinant N_2OR from *Stutzerimonas stutzeri* by modifying the last step of the purification procedure from the one published [2]. The purified enzyme was characterized by visible spectroscopy and CD. The activation mechanism of this enzyme was studied, showing that it can be activated through the incubation with reduced viologens (in the presence or absence of dithionite). The activated enzyme has a decay in activity upon removal of the reducing power, as observed for *Marinobacter nauticus* N_2OR [3]. The kinetic properties of the activated form are presented.

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Enhanced reduction of nitroarenes using MoS_2–LDH hybrid catalysts

P21

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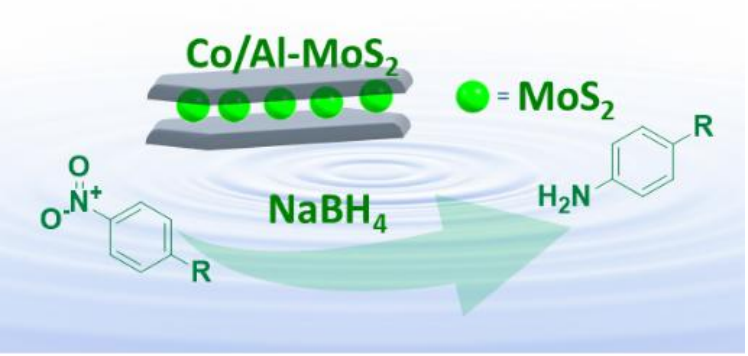
Aromatic amines are a class of compounds of high industrial importance.[1] One way to obtain these materials is through the hydrogenation of the corresponding nitro aromatic compound, however due to the use of noble metal catalysts and hydrogen in the catalytic reaction, the development of "greener" processes using more common and less toxic reagents has garnered much attention.[2]

Molybdenum disulfide (MoS_2) is a two-dimensional transition–metal dichalcogenide whose layered structure resembles graphene. Its unique electronic and catalytic properties have driven its application in several applications.[3] Another promising class of catalytic materials are Layered Double Hydroxides (LDHs), such as Co/Al LDH, which are valued for their tunability, stability, and low cost, and have been successfully applied in reduction reactions.[4]



In this study, MoS_2, Co/Al LDH, and a MoS_2–Co/Al LDH hybrid material were synthesized via a hydrothermal route. These materials were evaluated as catalysts for the reduction of nitroarenes using sodium borohydride as hydrogen source. Results show that MoS_2, MoS_2–Co/Al LDH, and Co/Al LDH–MoS_2 exhibit catalytic activity, whereas Co/Al LDH by itself is inactive under the tested conditions. The hybrid materials outperform the individual components, with MoS_2–Co/Al LDH showing enhanced activity at low reducing-agent concentration, and Co/Al LDH–MoS_2 present the highest overall activity.

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Mn-catalysts for CO_2 conversion into formic acid

P22

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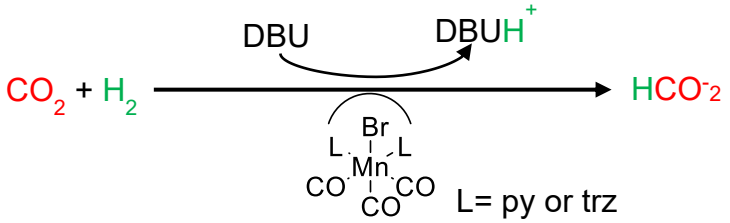
The unprecedented increase in atmospheric CO_2 levels is triggering severe and unpredictable negative impacts on climate and oceans. To halt these catastrophic events, it is urgent to develop efficient methods to decrease atmospheric CO_2 and use it in the production of *de novo* added-value products. In this context, converting CO_2 into formic acid (FA) presents a promising solution for carbon recycling, as FA can be reconverted into various added-value products for the energy and chemical industries [1]. To accomplish this, the chemical route of CO_2 reduction to FA has been widely explored, particularly CO_2 homogeneous hydrogenation. Typically, this reaction is catalyzed by different metal complexes. For instance, the catalytic performance of Mn complexes in acetonitrile is already reported in the literature [2].

In this work, we explored the base (DBU)-assisted CO_2 hydrogenation to FA catalyzed by Mn-based complexes (eq. 1). These bromo tricarbonyl Mn complexes are coordinated by either triazole (trz) or pyridine (py) ligands and were previously prepared and characterized [3]. The reaction conditions such as temperature, pressure, DBU concentration and catalyst amount were optimized. The aim is to develop a highly efficient and sustainable CO_2 conversion system, with high FA selectivity and conversion.



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3-Hydroxy-4-Pyridinones as chromogenic and fluorescent probes for metal ions

P23

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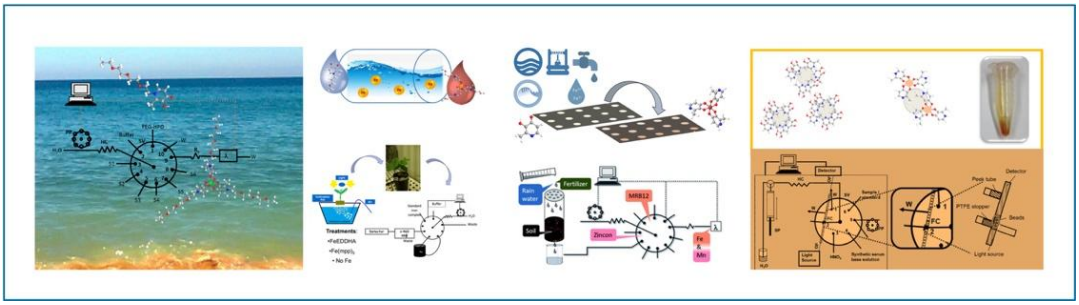
Chelators of the 3-hydroxy-4-pyridinone class are known for their chemical, biomedical, agricultural and environmental applications. The possibility of using the ligands in such a variety of fields is mainly due to their high affinity towards M(II) and M(III) metal ions and are versatile in chemical synthesis. A significant number of bidentate ligands with variable lipophilicity have been prepared and further used to synthesize polydentate ligands. Additional functionalities such as fluorophores and anchoring molecules to connect the chelating units to particular molecular frameworks have been successfully introduced thus enlarging their range of application.

An overview of the work developed in our laboratories regarding the design of ligands and studies of chemical properties and hydrophilic/lipophilic balance will be presented focusing on the application of 3-hydroxy-4-pyridinones in the quantification of metal ions in various matrices. [1]



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Advancing carbon neutrality: CO_2 utilisation using metal-organic frameworks

P24

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The escalating global warming crisis, driven by the excessive accumulation of atmospheric CO_2, needs the development of urgent mitigation strategies. While global agreements aim to limit temperature increases, CO_2 emissions are still projected to rise significantly due to growing energy demands. Consequently, carbon capture, sequestration, and subsequent conversion have become fundamental strategies for reducing atmospheric emissions. [1]

Among the most promising materials for these applications are Metal-Organic Frameworks (MOFs), crystalline porous compounds characterised by their immense structural variety, exceptionally high surface areas and high density of open metal sites. MOFs can be engineered for several catalytic reactions, namely the CO_2 electroconversion into high value-added chemical compounds (e.g. CH_3OH, HCOOH, CH_4, etc.) [1,2]

In this work, two families of MOFs are explored: modified Cu–purine MOFs[3] for CO_2 electroreduction, and MOF-74[1] for CO_2-based electrocarboxylation of organic substrates to carboxylic acids, in both cases relying on CO_2 adsorption within the MOF pores followed by electrochemical transformation. The performance of these systems is assessed under CO_2 atmosphere by bulk electrolysis, quantifying Faradaic efficiency, product selectivity and operational stability, with product analysis by gas chromatography with thermal conductivity detector and ^1H nuclear magnetic resonance spectroscopy.

These integrated approaches shift the perspective of CO_2 from an environmental pollutant to a valuable industrial resource.

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Biological effect of Ni(II)-polyamine complexes on lung cancer cells

P25

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Lung cancer is the highest mortality rate malignancy worldwide, with 15% of deaths associated to SCLC (small cell lung cancer) and 85% NSCLC (non-small cell lung cancer) [1,2]. Overall survival is substantially low, chemotherapy, being the standard treatment by combined administration of a platinum agent (cisplatin or carboplatin) with a third-generation drug. However, its efficacy is constrained by severe side effects and acquired resistance [3]. New anticancer agents are thus an unmet clinical need. Metal complexes with biogenic polyamines have been studied by the team [4,5]. The present work focuses on two Ni(II)-spermidine (Spd)/spermine (Spm) complexes: $Ni_3(NH_2(CH_2)_3NH(_CH_2)_4NH)_3Cl_6$ (Ni_3Spd_2) and $Ni_2NH_2(CH_2)_3NH(CH_2)_4NH(CH_2)_3NHCl_4$ (Ni_2Spm). Their effect on cell proliferation was assessed on H69 and A549 human lung cells and compared with cisplatin. Ni_2Spm and cisplatin showed a dose-dependent reduction on cell growth, at 72 h of drug exposure (Fig. 1).

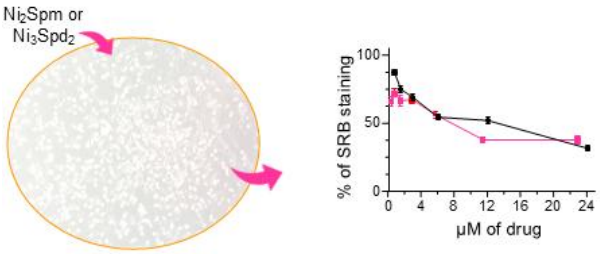

Figure 2 - Graphical abstract

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Light-sensitive cationic porphyrin-films for photoinactivation of MDR bacteria

P26

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Infections caused by multidrug-resistant (MDR) microorganisms represent a major challenge in modern medicine and place a substantial burden on healthcare systems worldwide. A key contributor to the spread of MDR bacteria is contact with contaminated hospital surfaces and medical devices, which can rapidly lead to severe and potentially life-threatening infections [1,2]. To address this issue, the development of broad-spectrum antimicrobial surfaces capable of inactivating bacteria upon contact, reducing pathogenicity, and preventing biofilm formation is essential. One promising approach involves the use of photosensitive materials[3,4], that combine a polymeric matrix—preferably based on biodegradable biopolymers—with embedded photosensitizers (PS), **Figure 1**. Cationic imidazolium-substituted porphyrins are among the most promising photosensitizers for such materials due to their high stability, favorable photophysical and photochemical properties, and broad-spectrum antimicrobial activity [5]. In this study, we report the synthesis and characterization of novel cationic imidazolium porphyrins and their incorporation into polylactic acid (PLA)-based photosensitive materials. The resulting biopolymer–photosensitizer composites exhibited complete photoinactivation (7-log reduction) of both Gram-positive and Gram-negative bacteria under blue light irradiation, highlighting the critical role of photosensitizer amphiphilicity in material stability and antibacterial efficacy.

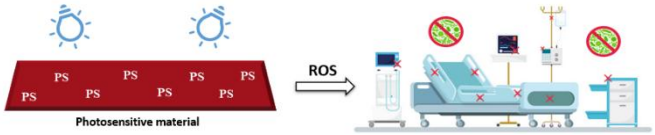

Fig. 1. Schematic overview of the process of photodecontamination of surfaces.

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Graphene-enzymatic nanohybrid for sustainable water purification

P27

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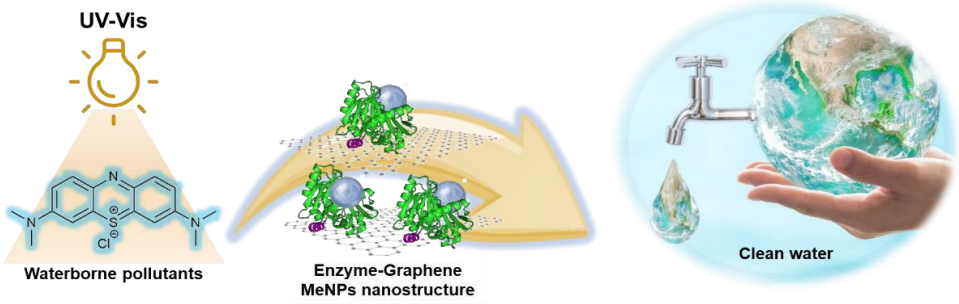

Water contamination by persistent organic pollutants requires sustainable and efficient remediation strategies. Graphene-based materials are promising photocatalysts for water treatment due to their high surface area and ability to enhance interfacial charge transfer [1,2]. However, conventional graphene production often relies on oxidative routes involving toxic reagents and harsh conditions.

Herein, we report a green, enzyme-assisted strategy to synthesize graphene–metal oxide bionanohybrids in aqueous media, following previously reported methods [3]. Few-layer graphene was obtained via ultrasound-assisted liquid-phase exfoliation of graphite combined with immobilized microbial lipases, including *Candida antarctica* lipase B (CALB) and *Thermomyces lanuginosus* lipase (TLL), which act as bio-stabilizing agents. Photocatalytically active metal oxide nanoparticles were subsequently generated *in situ* on the graphene surface, forming enzyme-mediated hybrid nanostructures.

The photocatalytic performance of these materials is currently being assessed for the degradation of waterborne contaminants. Preliminary adsorption tests (10 ppm pollutant, 2.5 mg catalyst, 60 min) reveal only minor adsorption, markedly lower than that of commercial functionalized graphene (typically 2–6 $mg \cdot g^{-1}$ at pH ≈ 7). Even so, the hybrid architecture promotes controlled nanoparticle growth and well-defined catalytic interfaces, underscoring the promise of enzyme-mediated graphene hybrids as sustainable platforms for water remediation.

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EXPLORING NEW ROLES IN SNAP-TAG SYSTEMS

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P28

The SNAP-tag is a protein labeling system that exploits the specificity of O6-alkylguanine-DNA alkyltransferase (AGT) to enable covalent conjugation between a labelled substrate and a target protein.[1] Although it is widely used for intracellular protein tracking, the labelling reaction typically generates guanine as a by-product.[2] We aim to extend the utility of this by-product by chemically functionalizing guanine to serve dual roles: as a potential anticancer agent and as a vector for targeted delivery, enabling mechanistic insight into its mode of action.

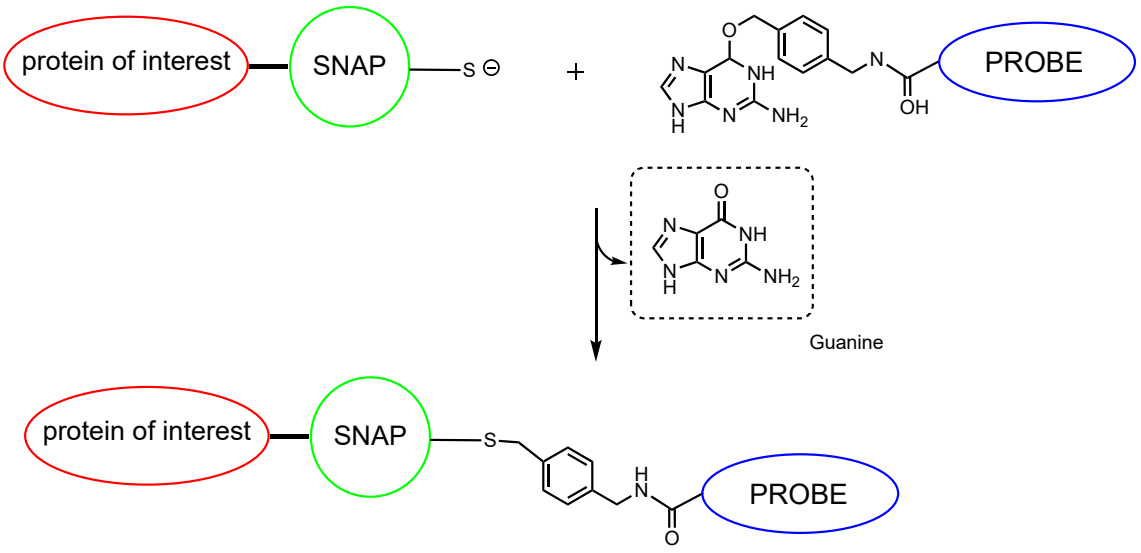

Figure 3

We are currently working to understand how halogenation and subsequent metalation influence the reactivity of guanine derivatives while preserving their selective labelling by the SNAP-tag enzyme. In line with this, we have examined several synthetic methods for the preparation of SNAP-TAG precursors and the results will be discussed in this communication.

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