

scientific output indicators

2024

Overall Output Indicators

2024
by group

	SM	MC	CCST	OC	BC	Total*
Books / Book Chapters	37	3	9	3	4	56
Articles in International Journals	60	39	43	25	28	175
Articles in National Journals	1	1	1	1	-	4
Communications at International Meetings	59	45	33	28	17	169
Communications at National Meetings	19	17	17	24	23	86
Conferences / Seminars Organization	13	5	7	4	4	35
Thesis (PhD + MSc + BSc)	26	16	23	26	6	95
Reports	1	1	1	-	-	3
Lab Prototypes / Software	-	1	-	-	-	1
Patents	5	1	1	2	-	9
Conferences Proceedings	3	1	7	1	1	13
Awards and Distinctions	2	2	6	4	3	15

*Adjusted Total, excluding groups collaborations

SM_ Soft Matter
 MC_ Medicinal Chemistry
 CCST_ Computational Chemistry Spectroscopy & Thermodynamics
 OC_ Organic Chemistry
 BC_ Biological Chemistry

Contents

	Page
Books and Book Chapters.....	3
Articles in International Peer-Reviewed Journals.....	8
Articles in National Peer-Reviewed Journals.....	22
Communications at International Meetings.....	23
Communications at National Meetings.....	37
Conferences and Seminars Organization.....	45
Thesis Mentorship	47
Technical Reports.....	57
Lab Prototypes / Software.....	55
Patents.....	55
Conferences Proceedings.....	57
Awards and Distinctions	59

Books and Book Chapters (56)

1. Ribeiro, A.C.F., Haghi, A.K., *Smart Water Resource Management: A Practical Introduction (Synthesis Lectures on Emerging Engineering Technologies)*, 1st Edition, Springer, 2024.
ISBN:13 978-303-16-0798-1
2. Ribeiro, A.C.F., Haghi, A.K., *Internet of Things (IoT) and Wastewater Reuse*, 1st Edition, Kindle Edition, RIVER PUBLISHERS, 2024.
ISBN: 9788770042208
3. Kulkarni, S., Haghi, A.K., Manwatkar, S., *Novel Technologies in Biosystems, Biomedical & Drug Delivery*, Ed. I, Springer 2024.
ISBN: 978-981-99-5280-9. DOI: 10.1007/978-981-99-5281-6
4. Kulkarni, S., Kharisov, B., Haghi, A. K., Srivastava, V., *Next Generation Materials for Sustainable Engineering"*. Ed. I, IGI 2024.
ISBN: 979-836--9313-060., DOI: 10.4018/979-8-3693-1306-0
5. Kulkarni, S., Haghi, A.K., *Global Sustainability: Trends, Challenges & Case Studies*, Ed. I, Springer 2024.
ISBN: 978-303-1574-559
6. Kulkarni, S., Haghi, A.K., Manwatkar, S., *Biosystems, Biomedical & Drug Delivery Systems: Characterization, Restoration and Optimization*, Ed. I, Springer 2024.
ISBN: 978-981-97-2595-3
7. Kulkarni, S., Akolkar, H., Vijaykar, Haghi, A.K., *S-Heterocycles: Retrospect, Prospects, and Biological Applications*, Ed. I, Royal Society of Chemistry 2024.
ISBN: 978-183-76-7401-5
8. Kulkarni, S., Haghi, A.K., Yingngam, B., Ogwu, M., *Medical Applications of Biocompatible Surfaces and Coating*, Ed. I, Royal Society of Chemistry 2024.
ISBN: 978-183-76-7434-3
9. Kulkarni, S., Bhandari, S. V., Yingngam, B., Haghi, A.K., *Green Chemistry for Sustainable Engineering*, Ed. I, Cambridge Scholars Publishing 2024.
ISBN: 978-1-0364-0716-2.
10. Parray, J.A., Haghi, A.K., Meraj, G., *IoT-Based Models for Sustainable Environmental Management*, Ed. I, Springer 2024.
ISBN: 978-303-1743-733.
11. Parray, J.A., Gunjal, A., Shameem, O., Haghi, A.K., *Microplastics Pollution Control in Water Systems: Practical Solutions*, Ed. I, Springer 2024.
ISBN: 978-303-1743-986.
12. Yaser, A.Z., Samah, M.A.A., Ariffin, F., Haghi, A.K., *Controlling Environmental Pollution: Practical Solutions*, Ed. I, Springer 2024.
ISBN: 978-981-9789-306
13. Parray, J.A., Shameem, N., Haghi, A.K., *Environmental Landscape and Sustainable Biodiversity for Healthy Green Growth*, Ed. I, Springer 2024.
ISBN: 978-303-1754-043
14. Deka, S.C., Nickhil C., Haghi, A. K. *Engineering Solutions for Sustainable Food and Dairy Production: Innovations and Techniques in Food Processing and Dairy Engineering*, Ed. I, Springer 2024.
ISBN: 978-303-1754-331
15. Talukder, M., Kumar, S., Haghi, A. K., *Application of Waste-to-Energy Innovations in Tourism*, Ed. I, IGI 2024.

CQC – Overall Output Indicators 2024

ISBN: 979-836-9376-058

16. Albattat, A., Singh, A., Tyagi, P.K., Haghi, A. K., *Solid Waste Management and Disposal Practices in Rural Tourism*, Ed. I, IGI 2024.

ISBN: 979-836-9396-216

17. Yingngam, B., Aslam, M.S., Haghi, A.K., *Sustainable Pharmaceutical Product Development and Optimization Processes: From Eco-Design to Supply Chain Integrity*, Springer 2024.

ISBN: 978-9819797066

18. Dutta, P.K., Hamad, A., Haghi, A. K., Prabhakar, P.K., *Food and Industry 5.0: Transforming the Food System for a Sustainable Future*, Ed. I, Springer 2024.

ISBN: 978-303-17-6757-9

19. Albattat, A., Singh, A., Tyagi, P.K., Haghi, A.K. *Solid Waste Management for Rural Regions*, Ed. I, IGI 2024.

ISBN: 979-836-9385-272

20. Parray, J.A., Shameem, N., Haghi, A.K., *Sustainable Urban Environment and Waste Management: Theory and Practice*, Ed. I, Springer 2024.

ISBN: 978-981-9611-393~

21. Parray, J.A., Shameem, N., Haghi, A.K., *Management of Waste to Control Environmental Pollutions: Sustainability and Economic Feasibility*, Ed. I, Springer 2024.

ISBN: 978-303-1808-449

22 Parray, J.A., Shameem, N., Haghi, A.K., *Producing Healthy Food with Healthy Soils: Hazardous Waste Management*, Ed. I, Springer 2024.

ISBN: 978-303-1825-354

23. Thaichon, P., Dutta, P.K., Haghi, A. K., Dutta, S., *Digital Disruption in Hospitality, Sustainable Hospitality: A Global Perspective on People, Planet, and Profit*, Ed. I, Emerald Publishing 2024.

ISBN: 978-183-6623-618

24. Thaichon, P., Dutta, P.K., Haghi, A. K., Dutta, S., *Digital Disruption in Hospitality, AI and Emerging Technologies: A Roadmap to Personalized Experiences, Enhanced Operations, and Revenue Growth*, Ed. I, Emerald Publishing 2024.

ISBN: 978-183-6087-977

25. Kulkarni, S. Haghi, A.K., Egbuchunam, T.O., Kakodkar, S., *Hospital Waste Management and Toxicity Evaluation*, Ed. I, IGI, 2024.

ISBN: 979-836-93-5757-6., DOI: 10.4018/979-8-3693-5757-6

26. Parray, J.A., Mir, M.Y., Haghi, A.K., *Enzymes in Environmental Management*, Ed. I, Springer 2024. ISBN: 978-303-1748-738

27. Parray, J.A., Singh, N., Haghi, A.K., *Microalgae as a Sustainable Source of Green Energy Generation and Bioeconomy*, Ed. I, Springer 2024.

ISBN: 978-303-1777-028

28. Shaheemath Suhara K. K., Haghi, A.K., *GIS in Environmental Engineering: Core Concepts for Sustainable Development*, Ed. I, Springer 2024.

ISBN: 978-3-031-79125-3

29. Parray, J.A., Mir, M.Y., Shafi. N., Haghi, A.K., *Ozone Technology for Food Processing and Preservation*, Ed. I, Springer 2024.

ISBN: 978-303-1814-600

30. Talukder, M., Haghi, A. K., Khan, M., *Empowering Local Communities through Blockchain Tourism Initiatives*, In: *Exploring the World with Blockchain Cryptotravel* (pp. 000-000), IGI, 2024.

31. Aggarwal, S., Jain, R., Agarwal, A., Saxena, S., Haghi, A. K, *Computer-assisted Analysis of Proteomics and Genomics*, In: *Computer-Assisted Analysis for Digital Medicinal Imagery* (pp. 167-182), IGI 2024
ISBN:979-836-9352-267
32. Talukder, M., Kabir, F., Haghi, A.K, *Artificial Intelligence in the fields of Financial Management and Hospitality*, , In: *Utilizing AI and Machine Learning in Financial Analysis* (pp. -), ISBN: 979-836-9385-081, IGI 2024
33. Fernandes, F.R.L., Ribeiro, A.C.F., *Diffusion in Aqueous Electrolyte Solutions in Clinical and Pharmaceutical Research: Concepts, Models, and Its Impact in Scientific Community*, in “Pharmaceutical Science & Technology, Micro- and Nanoscale Technologies in Drug DeliveryA Contemporary Chemical Approach”, Eds. A.C.F. Ribeiro, A.R. Abraham, A.K. Haghi, Chapter 13, Apple Academic Press, Inc./CRC Press, New Jersey. In press.
34. Marques, J.M.C., *Modeling Microsolvation Features Involving Clusters*, in *Comprehensive Computational Chemistry*, M. Yáñez and R. J. Boyd (eds.), Elsevier, Oxford, vol. 2, pp 509-522, 2024.
ISBN: 978-0-12-823256-9
35. Santos, C. I. A. V, Barros, M. C. F., Mialdun, A., Shevtsova, V. Ribeiro, A. C. F., *Critical assessment and consistent parametrization of Fickian diffusion in mixtures of toluene, methanol and cyclohexane*, *Physics and Mechanics of New Materials Synthesis, Processing, and Emerging Applications*. United States: CRC Press, Apple Academic Press, 2024
ISBN: 9781774915738
E-Book ISBN: 9781003487760
36. Santos, C. I. A. V, *Ciência para Todos - Manual de atividades de ciência experimental para crianças*. Universidade de Coimbra, Portugal. 2024.
37. Pais, A., Cova, T.; Nunes, S., Vitorino, C., *Artificial Intelligence for Drug Product Lifecycle Applications*, Elsevier, 2024.
eBook ISBN: 9780323972512
<https://doi.org/10.1016/C2021-0-01352-3>
38. Pereira, M.M., Carrilho, R.M.B., Rodrigues, F.M.S., Dias, L.D.; Calvete, M.J.F., *Hydroformylation Catalysts for the Synthesis of Fine Chemicals*, em “*Catalysis for a Sustainable Environment*” (Ed. A.J.L. Pombeiro; M. Sutradhar; E.C.B.A. Alegria) John Wiley and Sons Ltd, 2024, Volume 2, Cap. 14, pp. 301-322.
ISBN (Impresso): 978-1-119-87052-4; eISBN (pdf): 978-1-119-87063-0
39. Pereira, M.M., Pinto, S.M.A., Dias, L.D., *Pyrrrole based Bioconjugates: An Experimental Approach*, CRC Press – Taylor & Francis Group (Boca Raton, USA), 2024, pp 1-124
ISBN (Impresso): 9780367634575 (print book); eISBN: 9781003119265.
40. Pereira, M.M., Carrilho, R.M.B., Calvete, M.J.F. *Tervalent Phosphorus Acid Derivatives emOrganophosphorus Chemistry Volume 52-Specialist Periodical Reports Series*; Editors: David W Allen, David Loakes and John C Tebby, Royal Society of Chemistry Books, Cambridge, 2024, 52, 1-25.
<https://doi.org/10.1039/BK9781837672738-00001>
41. *Molecules* (Special issue: “*Molecular Spectroscopy and Molecular Structure: Commemorative Issue in Honor of Professor Austin J. Barnes on Occasion of his 75th Birthday*”), Eds. R. Fausto, S. Turrell and G. O. Ildiz, MDPI, Basel (Switzerland), 2024, ISBN 978-3-7258-1851-8, 2024.
DOI: 10.3390/books978-3-7258-1851-8
42. *Photochem* (Special issue: “*Theme Issue in Honor of Prof. Maciej J. Nowak, for His Contributions to the Field of Photochemistry of Matrix-Isolated Species*”), Eds. R. Fausto and R. Kólos, MDPI, Basel (Switzerland), 2021. 2024 ISBN 978-3-7258-1851-8, ISBN978-3-7258-1210-3 (Hardback), ISBN978-3-7258-1209-7 (PDF).
DOI: 10.3390/books978-3-7258-1209-7
43. *Photochem* (Special issue: “*Feature Papers in Photochemistry II*”), Eds. R. Fausto, M. Guzman and V. Vaiano. MDPI, Basel (Switzerland), 2024.

URL: https://www.mdpi.com/journal/photochem/special_issues/8PJ9ODE8VG

44. Marques, U. F., Filipe, S., Catarino, H., Nogueira, B. A., Fausto, R., *Identification of Decorative Pigments in Ceramic and Stone Artefacts from Late Antiquity, Islamic Period and Modern Age belonging to the Archaeological Collection of the Rectory of the University of Coimbra, by Raman Spectroscopy* in “Current Approaches, Solutions and Practices in Conservation of Cultural Heritage”, (Eds. E. Gulder, A. Yilmaz, G. O. Ildiz, P. Pogliani and R. Fausto, Istanbul University Press, 2024. ISBN: 978-605-07-1592-7
URL: <https://iupress.istanbul.edu.tr/tr/book/current-approaches-solutions-and-practices-in-conservation-of-cultural-heritage/home>
45. *Molecules* (Special Issue: “From Spectroscopic Insights to Structural Wonders: A Theme Issue Dedicated to Professor Jaan Laane”), Eds. R. Fausto and G. Ogruc Ildiz, MDPI, Basel (Switzerland), 2024.
URL: https://www.mdpi.com/journal/molecules/special_issues/Professor_Jaan_Laane
46. *Spectroscopy Journal* (Special Issue: “Vibrational Spectroscopy and Biospectroscopy: Commemorative Issue Saluting the Pioneering Contributions of Prof. Henry Mantsch”), Eds. R. Fausto and S. Turrell, MDPI, Basel (Switzerland), 2024.
URL: https://www.mdpi.com/journal/spectroscj/special_issues/I0EICD24Q0
47. *European Physics Journal* (Special Issue: “Materials Development for the Circular Economy at Scientific Infrastructures”), Eds. S. Facsko, M. Stuckelberger, R. Fausto, J. Drnec, R. Dunin-Borkowski, P. King and G. García. Springer, Berlin (Germany), 2024.
48. *Photochem* (Special issue: “Photochemistry of Organic Molecules and of Matrix-Isolated Reactive Intermediates: Themed Issue Honoring Professor Rui Fausto for His Contributions to the Field”), Eds. G.O. Ildiz and L. L. G. Justino, MDPI, Basel (Switzerland), 2024. ISBN 978-3-7258-2604-9 (Hardback), ISBN 978-3-7258-2603-2 (PDF).
DOI: 10.3390/books978-3-7258-2603-2
49. Duque-Prata, Serpa, C., Caridade, P.J.S.B. *Properties of Charge Transfer States Based on (TD)-DFT: Defying Accuracy* in *Density Functional Theory: Fundamental Theory, Key Methods, and Applications*, A.E. Kuznetsov (Ed), (Elsevier, Chapter 15, in press).
50. Alves, A. J. S., Laranjo, M., Botelho, M. F., Pinho e Melo, T. M. V. D., Pineiro, M., Photodynamic therapy for skin wound healing: the role of porphyrin type photosensitizers, em “*Drug Delivery Systems for Wound Healing*”, (Ed. P. Fonte e P. Brandão), Elsevier, 2024, Volume 1, Cap. 11, pp.305-336.
ISBN (impresso) 9780323858403; eISBN: 9780323900812
51. Amorim, A. C., Burke, A. J. Supported Chiral Organocatalysts for Accessing Fine Chemicals in Catalysis for a Sustainable Environment, em “Catalysis for a Sustainable Environment”, (Eds. A. Pombeiro, E. Alegria, M. Sutradhar), Wiley, 2024, Cap. 29, pp. 639-657.
ISBN (impresso): 9781119870524
<https://doi.org/10.1002/9781119870647.ch29>
52. Moutayakine, A., Burke, A. J. Catalytic Routes to 1,2,3-Triazoles: New Developments and Applications, em “Synthesis and Applications in Chemistry and Materials”, como parte de *Chemistry, Energy and the Environment* (Eds. A. Pombeiro, F. Guedes, K. Mahmudov), World Scientific, 2024, Cap. 17, pp. 161-183.
ISBN (impresso): 978-981-12-7993-5; eISBN: 978-981-12-7995-9
https://doi.org/10.1142/9789811283215_0017
53. Carniato, F., Tei, L., Geraldes, C.F.G.C., *Manganese and Iron Based Nanoparticles as MRI Contrast Agents, em “Lanthanides and Other Transition Metal Ion Complexes and Nanoparticles in Magnetic Resonance Imaging”*, (Ed. C.F.G.C. Geraldes), CRC Press (Boca Raton, FL, EUA), 2024, Cap. 11, pp. 327-366.
ISBN (Impresso) 978-1-03243-836-8; eISBN (pdf): 978-1-00337-468-8.
54. Cerofolini, L., Silva, J.M., Ravera, E., Fragai, M., Macedo, A.L., Parigi, G., Geraldes, C.F.G.C., *Paramagnetic NMR of Transition Metal Derivatives of Human Carbonic Anhydrase: Implications for Enzyme Catalysis and Sustainability*, in “*Synthesis and Applications in Chemistry and Materials - Volume 12: Enzymatic and Organic Systems, Part IV — Enzymatic and Related Systems and Materials*”, (Ed. A.J.L. Pombeiro, K.T. Mahmudov, M.F.C. Guedes da Silva), World Scientific Publishing Company (Singapore), 2024, Cap. 11, pp. 39-78.

CQC – Overall Output Indicators 2024

ISBN: 978-981-12-7994-2

ISBN (Impresso) 978-981-12-7993-5; eISBN (pdf): 978-981-12-7995-9.

55. Geraldés, C.F.G.C. (Editor), *Lanthanides and Other Transition Metal Ion Complexes and Nanoparticles in Magnetic Resonance Imaging*, CRC Press (Boca Raton, FL, EUA), 2024.

ISBN (Impresso) 978-1-03243-836-8; eISBN (pdf): 978-1-00337-468-8.

56. Machado, F., Coimbra A., M., Coreta-Gomes, F., *Coffee dietary fiber: features and hypocholesterolemic effects*, in “*Coffee in Health and Disease Prevention*”, (Ed. V.R. Preedy, V.B. Patel), 2.^a edição, Academic Press (Londres, Reino Unido), 2024., Cap. 25, pp. 277-285.

ISBN 978-0-44313-868-3; eISBN (pdf): 978-0-44313-869-0.

Articles in International Peer-Reviewed Journals (175)

1. Rodrigo, M. M., Cabral, A. M. T. D. P. V., Fangaia, S. I. G., Afonso C. Nogueira, A. C., Valente, A. J. M., Ribeiro, A. C. F., Estes, M. A., *On the Diffusion of Anti-Tuberculosis Drugs in Cyclodextrin-Containing Aqueous Solutions*, *Liquids*, 4(4), 702-709, 2024.
DOI: 10.3390/liquids4040039
2. Rodrigo, M. M., Fernandes, F. R. L., Fangaia, S. I. G., Crespo, A., Ribeiro, A. C. F., Estes, M. A., *Coupled Transport of Metal Ions in Aqueous Solutions Containing NaCl and HCl*, *Inorganics*, 12(10), 259, 2024.
DOI:10.3390/inorganics12100259
3. Fangaia, S. I. G., Messias, A., Guerra, F. A. D. R. A., Ribeiro, A. C. F., Valente, A. J. M., Nicolau, P. M. G., *Evaluation of the Tribocorrosion Behavior of Ti-6Al-4V Biomedical Alloy in Simulated Oral Environments*, *Processes*, 12(7), 1283, 2024.
DOI:10.3390/pr12071283
4. Vareda, J. P., Fonseca, A. C., Ribeiro, A. C. F., Pontinha, A. D. R., *Silica-Poly(Vinyl Alcohol) Composite Aerogel: A Promising Electrolyte for Solid-State Sodium Batteries*, *Gels*, 10(5), 293, 2024.
DOI:10.3390/gels10050293
5. Fangaia, S. I. G., Silva, D. S. A., Messias, A., Nicolau, P. M. G., Valente, A. J. M., Rodrigo, M. M., Ribeiro, A. C. F., *Transport Properties in Multicomponent Systems Containing Cyclodextrins and Nickel Ions*, *Int. J. Mol. Sci.*, 25(8), 4328, 2024.
DOI: 10.3390/ijms25084328
6. Sofio, S. P. C., Caeiro, A., Ribeiro, A. C. F., Cabral, A. M. T. D. P. V., Valente, A. J. M., Canhoto, J., Estes, M. A., *On Interactions of Sulfamerazine with Cyclodextrins from Coupled Diffusometry and Toxicity Tests*, *Biomolecules*, 14(4), 462, 2024.
DOI: 10.3390/biom14040462
7. Fernandes, F. R. L., F.R.G. Soares, S. F. R., Ribeiro, A. C. F., *Effect of Caffeine in the Diffusion Behaviour of Analgesic Drugs in Aqueous Solutions*, *Innovation Discovery*, 1(1), 6, 2024.
DOI: 10.53964/id.2024006.
8. Peixoto, L. O. M., Pereira, J. C., Fernandes, C. V. S., Centeno, J. A. S., Azevedo, J. C. R., *Modeling and Predicting Caffeine Contamination in Surface Waters Using Artificial Intelligence and Standard Statistical Methods*, *Environ. Monit. Assess.* 197, 30.
DOI: 10.1007/s10661-024-13423-2
9. Silva, E. C., Gomes, C. G., Pina, J., Pereira, R. F. P., Murtinho, D., Fajardo, A. R., Valente, A. J. M., *Carbon quantum dots-containing poly(β -cyclodextrin) for simultaneous removal and detection of metal ions from water*, *Carbohydrate Polymers*, 323, 121464, 2024.
DOI:10.1016/j.carbpol.2023.121464
10. Machado T. F., Utzeri, G., Valente, A. J. M., Serra, M. E. S., Murtinho, D., *Click Nanosponge – A Novel Amine-Rich β -Cyclodextrin-Based Crosslinked Polymer for Heterogeneous Catalysis*, *Carbohydrate Polymers*, 326, 121612, 2024.
DOI:10.1016/j.carbpol.2023.121612
11. Melro, E., Duarte, H., Eivazi, A., Costa, C., Faleiro, M. L., Costa, A. R., Antunes, F. E., Valente, A. J. M., Romano, A., Norgren, M., Medronho, B., *Poly(butylene succinate)-based composites with technical and extracted lignins from wood residues*, *ACS Applied Polymer Materials*, 6, 1169-1181, 2024.
DOI:10.1021/acscapm.3c02103
12. Miron, A., Iordache, T.-V., Valente, A. J. M., Durães, L. M. R., Sarbu, A., Ivan, G., Zaharia, A., Sandu, T., Iovu, H., Chiriac, A.-L., *Chitosan-Based Beads Incorporating Inorganic-Organic Composites for Copper Ions Retention in Aqueous Solutions*, *Int. J. Mol. Sci.*, 25(4), 2411, 2024.
DOI:10.3390/ijms25042411

13. Machado T. F., Valente, A. J. M., Serra, M. E. S., Murtinho, D., *Triazene-Linked Porous Organic Polymers for Heterogeneous Catalysis and Pollutant Adsorption*, ACS Applied Polymer Materials, 6, 4171–4185, 2024.
DOI:10.1021/acspapm.4c00225
14. Vareda, J. P., Matias, P. M. C., Paixão, J. A., Murtinho, D., Valente, A. J. M., Durães, L., *Chitosan-silica composite aerogel for the adsorption of cupric ions*, Gels, 10(3), 192, 2024.
DOI:10.3390/gels10030192
15. Silva, E. C., Pina, J., Pereira, R. F. P., Murtinho, D., Valente, A. J. M., Fajardo, A. R., *Synthesis and characterization of fluorescent poly(α -cyclodextrin)/carbon quantum dots composite for efficient removal and detection of toluene and xylene from aqueous media*, Environmental Pollution, 347, 123778, 2024.
<https://doi.org/10.1016/j.envpol.2024.123778>
16. Utzeri, G., Guirado-Moreno, J., Cova, T., Pais, A., Carvalho, L. B., Ibeas, S., Garcia, J., Valente, A. J. M., Vallejos, S., *Reusable and Effective Polyacrylic Membranes for Mecoprop and Bentazon Extraction*, npj Clean Water, 7, 39, 2024.
DOI:10.1038/s41545-024-00328-3
17. Matsushita, A., Pais, A. A. C. C., Valente, A. J. M., *Enhanced Luminescent Properties of Poly(sodium acrylate)-Based Composite And Its Selective Interaction Towards Copper Ions*, Optical Materials, 152, 115530, 2024.
DOI:10.1016/j.optmat.2024.115530
18. Guembe-Garcia, M., Utzeri, G., Valente, A. J. M., Ibeas, S., Trigo, M., García, J. M., Vallejo, S., *Efficient Extraction of Textile Dyes Using Reusable Acrylic-Based Smart Polymers*, Journal of Hazardous Materials, 476, 135006, 2024.
DOI:10.1016/j.jhazmat.2024.135006
19. Santos, J.A., Valente, A. J. M., Muniz, E. C., *Poly(vinyl alcohol) (PVA) for gene delivery: a systematic review*, Journal of Drug Delivery Science and Technology, 106149, 2024.
DOI:10.1016/j.jddst.2024.106149
20. Matias, P. M. C., Rodrigues, A. C. B., Nunes, S. C. C., Pais, A. A. C. C., Murtinho, D., Valente, A. J. M., *Assessing interactions between antibiotics and triazine porous organic polymeric sorbents by photophysics*, Environmental Pollution, 363, 125197, 2024.
DOI:10.1016/j.envpol.2024.125197
21. Duarte, H., Brás, J., Hassani, M. S., Gonzalez, M. J. A., Magalhães, S., Alves, L Valente, A. J. M., Eivazi, A., Norgren, M., Romano, A., Medronho, B., *Lignin-furanic rigid foams: Enhanced methylene blue removal capacity, recyclability, and flame retardancy*, Polymers, 16, 3315, 2024.
DOI:10.3390/polym16233315
22. Campos, M. G., Chia, M., Claudio, M, Capinha, M, Torres, R., Oliveira, S, Fortuna, A., *Potential Drug Interactions with Cannabinoids in selected Chronic Diseases: Epilepsy, Autism Spectrum Disorders, Oncology, Multiple Sclerosis and Pain*, Pharmaceuticals, 17(5),613, 2024.
DOI: 10.3390/ph17050613
23. Carona A, Bicker J, Fonseca C, Campos, M. G, Falcão, A, Fortuna, A., *Development and validation of an HPLC-DAD method for the quantification of cannabigerol, cannabidiol, cannabinol and cannabichromene in human plasma and mouse matrices*. Analyst., Jul 8,149(14), 3815-3827, 2024.
DOI: 10.1039/d4an00070f. PMID: 38847584.
24. Kacemi, R., Campos, M. G., *Translational Proofs on Bee Pollen Research for Neurodegenerative Diseases and Cancer as Source of BioPharmaceuticals*, Molecules, 29, 5893, 2024.
DOI: 10.3390/molecules29245893
25. Costa, B. D. P., Simões, J. C. S., Lopes, S. M. M., Laranjo, M., Rodrigues, A. C. B., Gonçalves, A. C., Seixas de Melo, J. S., M. F, Botelho, M. F., Pineiro, M., Pinho e Melo, T. M. V. D., *Hydrazone-Functionalized trans-A2B-Corroles: Effective Synergy in Photodynamic Therapy of Lung Cancer* Journal of Medicinal Chemistry, 67, 21934–21951, 2024.

DOI:10.1021/acs.jmedchem.4c01824

26. Cunha, C., Seixas de Melo, J. S., *From indigo to isoindigo: Rationalizing the high efficiency of photoprotective molecular mechanisms*, *Dyes and Pigments*, 229, 112307, 2024.

DOI:10.1016/j.dyepig.2024.112307

27. Cortés-Villena, A., Bellezza, D., Cunha, C., Rosa-Pardo, I., Seijas-Da Silva, A., Pina, J., Abellán, G., Seixas de Melo, J. S., Galian, R. E., Pérez-Prieto, J., *Engineering Metal Halide Perovskite Nanocrystals with BODIPY Dyes for Photosensitization and Photocatalytic Applications*, *Journal of the American Chemical Society*, 146, 14479–14492, 2024.

DOI:10.1021/jacs.3c14335

28. Cunha, C., Peixoto, M., Paixão, J. A., Pineiro, M., Seixas de Melo, J. S., *Tuning the AIE Properties of Di-tert-Butyl-diphenyldibenzofulvene Derivatives*, *The Journal of Physical Chemistry C*, 128, 1156–1164, 2024.

DOI:10.1021/acs.jpcc.3c06436

29. Pinheiro, D., Cunha, C., Pineiro, M., Galvão, A. M., Seixas de Melo, J. S., *Solvent-dependent ultrafast deactivation processes with phenylpropyl indigo derivatives: a step forward in the understanding of indigo decay mechanisms*, *Phys. Chem. Chem. Phys.*, 26, 28046–28054, 2024.

10.1039/D4CP03192J

30. Nobre, D. C., Delgado-Pinar, E., Cunha, C., Seixas de Melo, J. S., *The role of the oxime group in the excited state deactivation processes of indirubin*, *Phys. Chem. Chem. Phys.*, 26, 7416, 2024.

DOI:10.1039/D3CP05260E

31. Costa-Tuna, A., Chaves, O. A., Almeida, Z. L., Cunha, R. S., Pina, J., Serpa, C., *Profiling the Interaction between Human Serum Albumin and Clinically Relevant HIV Reverse Transcriptase Inhibitors*, *Viruses*, 16, 491, 2024.

DOI:10.3390/v16040491

32. Malta, G., Pina, J., Lima, J. C., Parola, A. J., Branco, P. S., *Acenaphthylene-Based Chromophores for Dye-Sensitized Solar Cells: Synthesis, Spectroscopic Properties, and Theoretical Calculations*, *ACS Omega*, 9, 1201, 2024.

DOI:10.1021/acsomega.4c01201

33. Benali, E. M., Saher, L., Benali, A., Bejar, M., Dhahri, E., Wu, J., Peng, L., Gordo, P. M., Pina, J., Costa, B. F. O., *Synthesis, characterization, and sensitivity tests of $La_{0.8}Ba_{0.1}Bi_{0.1}FeO_3$ nanoparticles towards a few parts-per-billion of acetone gas*, *Heliyon*, 10, e26778, 2024.

DOI:10.1016/j.heliyon.2024.e26778

34. Dhahri, A., Saoudi, H., Gavinho, S. R., Benali, A., Abdelmoula, N., Dhahri, R., Peng, L., Wu, J., Pina, J., Costa, B. F. O., *Particle Size Effect on Optical and Gas-Sensing Properties of $La_{0.67}Ca_{0.2}Ba_{0.13}Fe_{0.97}M_{0.03}O_3$ ($M = Ti^{4+}$, Mn^{3+} , and Cr^{3+}) Compounds*

Crystals, 14, 173, 2024.

DOI:10.3390/cryst14020173

35. Ben Ahmed, S., Pérez de Bustos, G., Pina, J., Torres, T., Rodríguez-Morgade, M. S., *Tuning Fluorescence and Singlet Oxygen Quantum Yields of Subporphyrazines by Axial Functionalization*, *Chem. Plus. Chem.*, 89, e202300779, 2024.

DOI:10.1002/cplu.202300779

36. Saadi, H., Khaldi, O., Pina, J., Costa, T., Seixas de Melo, J. S., Vilarinho, P., Benzarti, Z., *Effect of Co Doping on the Physical Properties and Organic Pollutant Photodegradation Efficiency of ZnO Nanoparticles for Environmental Applications*, *Nanomaterials*, 14, 122, 2024.

DOI:10.3390/nano14010122

37. Costa-Tuna, A., Chaves, O. A., Loureiro, R. J. S., Pinto, S., Pina, J., Serpa, C., *Interaction between a water-soluble anionic porphyrin and human serum albumin unexpectedly stimulates the aggregation of the photosensitizer at the surface of the albumin*, *Int. J. Biol. Macromol.*, 255, 128210, 2024.

DOI:10.1016/j.ijbiomac.2023.128210

38. Elhamdi, I., Souissi, H., Kammoun, S., Dhahri, E., Pina, J., Costa, B. F. O., López-Lago, E., *Comprehensive characterization and optoelectronic significance of Ho³⁺ and Cr³⁺ Co-doped ZnAl₂O₄ spinels*, Dalton Trans., 53, 198, 2024

DOI:10.1039/D4DT00198B

39. Almeida, Z. L., Cruz, P. F., Costa, T., Netto-Ferreira, J. C., de Lima, M. E. F., da Silva, M. B., Serpa, C., Chaves, O. A., *Lapachol, a natural food component, interacts with human serum albumin: Insights of its impact on the pharmacokinetics of clinically used drugs*, Int. J. Biol. Macromol, 282, 137520, 2024.

DOI:10.1016/j.ijbiomac.2024.137520

40. Cunha, R. S., Cruz, P. F., Costa, T., Almeida, Z. L., Lima, M. E. F., Serpa, C., Chaves, O. A., *Revisiting and Updating the Interaction between Human Serum Albumin and the Non-Steroidal Anti-Inflammatory Drugs Ketoprofen and Ketorolac*, Molecules, 29 (13), 3001, 2024.

DOI:10.3390/molecules29133001

41. Soares, M. A. G., de Aquino, P. A., Costa, T., Serpa, C., Chaves, O. A., *Insights into the effect of glucose on the binding between human serum albumin and the nonsteroidal anti-inflammatory drug nimesulide*, Int. J. Biol. Macromol, 265, 131148, 2024.

DOI:10.1016/j.ijbiomac.2024.131148

42. dos Santos, D. N. S., Naskar, N., Delgado-Pinar, E., Reess, K., Seixas de Melo, J. S., Rueck, A., *Bromine indirubin FLIM/PLIM sensors to measure oxygen in normoxic and hypoxic PDT conditions*, Photodiagnosis Photodyn. Ther., 45, 103964, 2024.

DOI:10.1016/j.pdpdt.2024.103964

43. Nunes Barradas, P. D.; Murtinho, D.; Sérgio Seixas de Melo, J., *Chitosan polymers randomly labeled with pyrene: synthesis, photophysics, and selective quenching by metal cations and anions*, J. Mol. Liq., 396, 123982, 2024.

DOI:j.molliq.2024.123982

44. Pinto, C. M., Clementi, C. Sabatini, F. Degano, I. Romani, A. Seixas de Melo, J. S. *Unveiling the photostability of the molecule of colour shikonin: From solution to solid state*, J.Mol. Struct., 1316, 138898, 2024.

DOI: 10.1016/j.molstruc.2024.138898

45. Zergani, F., Marques, J. M. C., Bartolomei, B., Pirani, F., *Borophene Nanoclusters: Energetics and Structures From Analytical Potentials*, J. Chem. Phys., 161(20), 204303, 2024.

DOI: 10.1063/5.0239149

46. Figueiredo, N. M., Voroshlyova, I. V., Ferreira, E. S. C., Marques, J. M. C., Fangaia, Cordeiro, M. N. D. S., *Magnetic Ionic Liquids: Current Achievements and Future Perspectives with a Focus on Computational Approaches*, Chem. Rev., 124(6), 3392-3415, 2024.

DOI: 10.1021/acs.chemrev.3c00678

47. Marques, J. M. C., Prudente, F. V., *Structure and thermodynamics of Li⁺Ar_n clusters beyond the second solvation shell*, Symmetry, 16(2), 229, 2024.

DOI: 10.3390/sym16020229

48. Encarnação, T., Nicolau, N., Ramos P., Silvestre, E., Mateus, A., Archer de Carvalho, T., Gaspar, F., Massano, A., Biscaia, S., Castro, R. A. E., Nogueira, B. A., Singh, P., Pacheco, D., Patrício, T., Fausto, R., Sobral A. J. F. N., *Recycling Ophthalmic Lens Wastewater in a Circular Economy Context: A Case Study with Microalgae Integration*, Materials, 17, 75, 2024.

DOI: 10.3390/ma17010075

49. Carmo, C., Almeida, J. M. S., Araújo, J., Brett, C. M. A., Botelho, M. F., Cordova, A., Laranjo, M., Sobral, A. J. F. N., *Exploring the impact of meso-position fluorination on BODIPYs: Synthesis, electrochemical Insights, and potential therapeutic applications in breast cancer*, Dyes and Pigments, 229, 112263, 2024.

DOI: 10.1016/j.dyepig.2024.112263

CQC – Overall Output Indicators 2024

50. Ojeda, G., Gil, J. M., Mattana, S., Bachmann, J., Quenea, K., Sobral, A. J. F. N., *Biochar ageing effects on soil respiration, biochar wettability and gaseous CO₂ adsorption*, *Mitig. Adapt. Strateg. Glob Change*, 29, 11, 2024.

DOI: 10.1007/s11027-024-10107-7

51. Braz, Sofia; Justino, Licinia L. G.; Ramos, M. Luisa; Fausto, Rui, *Indigo Carmine Binding to Cu(II) in Aqueous Solution and Solid State: Full Structural Characterization Using NMR, FTIR and UV/Vis Spectroscopies and DFT Calculations*, *Molecules* 29, 13, 3223, 2024. DOI:10.3390/molecules29133223.

52. Melro, E, Duarte, H., Eivazi, A., Costa, C., Faleiro, M., Costa, A., Antunes, FE, Valente, A., Romando, A., Norgren, M., Medronho, B., *Poly(butylene succinate)-Based Composites with Technical and Extracted Lignins from Wood Residue*, *ACS Applied Polymer Materials*, 6, 2, 1169-1191, 2024

DOI: 10.1021/acsapm.3c02103

53. Alves, L., Magalhaes, S., Esteves, C., Sebastião, M., Antunes, F., *Synergisms between Surfactants, Polymers, and Alcohols to Improve the Foamability of Mixed Systems*, *J*, 7, 2, 169-182, 2024

DOI: 10.3390/j7020010

54. Sousa, F., Jesus, C., Antunes, F., *Microcrystalline cellulose and by-products from the pulp and paper industry as reinforcing fibres for polybutylene succinate-based composites: A comparative study*, *Journal of Reinforced Plastics and Composites*, 43, 15-16, 912-925, 2024

DOI: 10.1177/07316844231198314

55. Mendes, M., Nunes, S., Cova, T., Branco, F., Dyrks, M., Kokschi, B., Vale, N., Sousa, J., Pais, A., Vitorino, C., *Charge-switchable cell-penetrating peptides for rerouting nanoparticles to glioblastoma treatment*, *Colloids and Surfaces B: Biointerfaces*, 241, 113983, 2024.

DOI: <https://doi.org/10.1016/j.colsurfb.2024.113983>.

56. Vigna, V., Cova, T. F. G. G., Nunes, S. C. C., Pais, A. A. C. C., Sicilia, E., *Machine Learning-Based Prediction of Reduction Potentials for Pt/IV Complexes*, *J. Chem. Inf. Model.*, 2024

DOI: 10.1021/acs.jcim.4c00315

57. Ribeiro, A., Montes, F., Sousa, J., Pais, A., *Comminution technologies in the pharmaceutical industry: a comprehensive review with recent advances*, *Reviews in Chemical Engineering*, 41, 1, pp. 69-100, 2024.

DOI: 10.1515/revce-2024-0059

58. Estes, M. A., Romero, C. M., *Cyclodextrins: Properties and Applications*, *Int. J. Mol. Sci.* 25, 4547, 2024.

DOI: 10.3390/ijms25084547

59. Maldonado-Sanabria, L. A., Rodriguez-Saavedra, I. N., Reyes-Peña, I. V., Castillo-Aguirre, A., Maldonado, M., Crespo, A., Estes, M. A., *Comparative study of the antioxidant activities of the conformers of C-tetra(4-methoxyphenyl)calix[4]resorcinarene*, *Int. J. Mol. Sci.* 25, 10010, 2024.

DOI: 10.3390/ijms251810010

60. Maldonado, M., Sanabria-Español, E., Romero, C. M., Galindres-Jiménez, D. M., Estes, M.A., *Study of the complexation of the stress hormone with (2-hydroxypropyl) α -, β - and γ -cyclodextrins in aqueous solution*, *Mol. Liquids* 415 (2024) 126386

DOI: 10.1016/j.molliq.2024.126386

61. M. Warszynska, B. Pucelik, C. S. Vinagreiro, P. Repetowski, A. Barzowska, D. Barczyk, F. A. Schaberle, A. Duque-Prata, L. G. Arnaut, M. M. Pereira, J. M. Dabrowski. "Better in the near infrared: Sulfonamide perfluorinated-phenyl photosensitizers for improved simultaneous targeted photodynamic therapy and real-time fluorescence imaging". *ACS Appl. Mat. Interfaces*, 16 (2024) 50389–50406.

DOI: 10.1021/acsami.4c11171

62. D. Vella, D. A. Pereira, A. Mrzel, D. Vengust, A. Drnovsek, L. G. Arnaut, C. Serpa, M. Jezersek. "Picosecond photoacoustic generation of ultrasounds with composites of graphene-decorated gold nanoparticles". *Nano Ene.*, 131 (2024) 110236

DOI: 10.1016/j.nanoen.2024.110236

63. A. S. Amorim, Z. A. Arnaut, A. I. Mata, B. Pucelik, A. Barzowska, G. J. da Silva, M. M. Pereira, J. M. Dabrowski, L. G. Arnaut “Efficient and selective, *in vitro* and *in vivo*, antimicrobial photodynamic therapy with a dicationic chlorin in combination with KI”. *ACS Infect. Dis.*, 10 (2024) 3368-3377.

DOI: 10.1021/acsinfecdis.4c00492

64. S. Melo-Guímaro, R. Cardoso, C. S. Lobo, D. A. Pereira, C. Varela, J. Santos, C. P. João, C. Serpa, L. G. Arnaut, “Delivery of monoxidil encapsulated in cyclodextrins with photoacoustic waves enhances hair growth”. *Eur. J. Pharm. Biopharm.*, 202 (2024) 114390.

DOI: 10.1016/j.ejpb.2024.114390

65. D. A. Mendonça, I. Cadima-Couto, C. C. Buga, Z. A. Arnaut, F. A. Schaberle, L. G. Arnaut, M. A. R. B. Castanho, C. Cruz-Oliveira, “Repurposing anti-cancer porphyrin derivative drugs to target SARS-Cov-2 envelope”. *Biomed. Pharmacother.*, 176 (2024) 116768.

DOI: 10.1016/j.biopha.2024.116768

66. M. F. C. Silva, R. T. Aroso, J. M. Dabrowski, B. Pucelik, A. Barzowska, G. J. da Silva, L. G. Arnaut, M. M. Pereira, “Photodynamic inactivation of *E. coli* with cationic imidazolyl-porphyrin photosensitizers and their synergic combination with antimicrobial cinnamaldehyde”. *Photochem. Photobiol. Sci.*, 23 (2024) 1129-1142.

DOI: 10.1007/s43630-024-00581-y

67. O.A. Chaves, D. Cesarin-Sobrinho, C. Serpa, M.B. Silva, M.E.F Lima, J.C. Netto-Ferreira, “The Presence of NSAIDs may Affect the Binding Capacity of Serum Albumin to the Natural Products Hymecromone and Umbelliferone”. *Int. J. Biol. Macromol.*, 283 (2024) 137981.

DOI: 10.1016/j.ijbiomac.2024.137981

68. Almeida, Z. L., Vaz, D. C., Brito, R. M. M., *Morphological and Molecular Profiling of Amyloid-β Species in Alzheimer’s Pathogenesis*, *Mol. Neurobiol.* 2024, 2024.

DOI: 10.1007/S12035-024-04543-4

69. O.A. Chaves, F.M. Martins, C. Serpa, D.F. Back, “The Role of Vanadium in Metallodrugs Design and Interactive Profile with Serum Albumin”. *Future Pharmacol.*, 4 (2024) 743-774.

DOI: 10.3390/futurepharmacol4040040

70. Geraldes, C.F.G.C., *Manganese Oxide Nanoparticles for MRI-Based Multimodal Imaging and Theranostics*, *Molecules*, 29, Art. N. 5591, 2024.

DOI: 10.3390/molecules29235591

71. L.A. Fontana, F.M. Martins, J.D. Siqueira, C. Serpa, O.A. Chaves, D.F. Back, “Synthesis of Cobalt (III) Complexes Derived from Pyridoxal: Structural Cleavage Evaluations and In Silico Calculations for Biological Targets”. *Inorganics*, 12 (2024) 171.

DOI: 10.3390/inorganics12060171

72. M.A.G Soares, F. Souza-Silva, C.R. Alves, L. Vazquez, T.S. Araujo, C. Serpa, O.A. Chaves, “Evidence of Hyperglycemic Levels Improving the Binding Capacity between Human Serum Albumin and the Antihypertensive Drug Hydrochlorothiazide”. *Sci. Pharm.* 92, (2024) 32.

DOI: 10.3390/scipharm92020032

73. D. Amado, O.A. Chaves, P.F. Cruz, R.J.S. Loureiro, Z.L. Almeida, C.S.H. Jesus, C. Serpa, R.M.M. Brito, “Folding Dynamics and Volume Variation of the β-Hairpin Peptide Chignolin upon Ultra-Fast pH-Jumps”. *J. Phys. Chem B*, 128 (2024) 4898-4910.

DOI: 10.1021/acs.jpcc.3c08271

74. M.L.S. Moreira, O.A. Chaves, N.C. Lucas, J. Goulart, S.J. Garden, C. Serpa, J.C. Netto-Ferreira, “Spectroscopic and in Silico Characterization of the Interaction between Synthetic 2-Substituted-Naphtho-1,4-quinones and Human Serum Albumin”. *J. Mol. Liq.*, 403 (2024) 124829.

DOI: 10.1016/j.molliq.2024.124829

75. M.A.G. Soares, P.A. Aquino, T. Costa, C. Serpa, O.A. Chaves, "Insights into the Effect of Glucose on the Binding between Human Serum Albumin and the Nonsteroidal Anti-inflammatory Drug Nimesulide". *Int. J. Biol. Macromol.*, 265 (2024) 131148.
DOI: 10.1016/j.ijbiomac.2024.131148
76. A. Duque-Prata, C. Serpa, P.J.S.B. Caridade, "Theoretical Evaluation of Fluorinated Resazurin Derivatives for In Vivo Applications". *Molecules*, 29 (2024) 1507.
DOI: 10.3390/molecules29071507
77. R.C. Ferreira, O.A. Chaves, C.H.C.S. de Oliveira, V. F. Ferreira, S.B. Ferreira, C. Serpa, D. Cesarin-Sobrinho, J. C. Netto-Ferreira, "Interactive Profile between 1,4-Naphthoquinone Derivatives and Human Serum Albumin". *J. Braz. Chem. Soc.*, 35 (2024) e-20240043, 1-11.
DOI: 10.21577/0103-5053.20240043
78. A. Costa-Tuna, O.A. Chaves, Z.L. Almeida, R.S. Cunha, J. Pina, C. Serpa, "Profiling the Interaction between Human Serum Albumin and Some Clinically Used Relevant HIV-Reverse Transcriptase Inhibitors". *Viruses*, 16 (2024) 491.
DOI: 10.3390/v16040491
79. O.A. Chaves, R.J.S. Loureiro, C. Serpa, P.F. Cruz, A.B.B. Ferreira, J.C. Netto-Ferreira, "Increasing the Polarity of β -Lapachone does not Affect its Binding Capacity with Bovine Plasma Protein". *Int. J. Biol. Macromol.*, 263 (2024) 130279.
DOI: 10.1016/j.ijbiomac.2024.130279
80. O.A. Chaves, C.H.C.S. Oliveira, R.C. Ferreira, V.F. Ferreira, S.B. Ferreira, C. Serpa, D. Cesarin-Sobrinho, F.A. Silva, J.C. Netto-Ferreira, "Spectroscopic and in Silico Evaluation on the Interactive Behavior between Substituted \square -2,3-Dihydrofuran Naphthoquinones and Human Serum Albumin". *Chem. Phys. Impact*, 8 (2024) 100465.
DOI: 10.1016/j.chphi.2024.100465
81. A. Costa-Tuna, O.A. Chaves, R.J.S. Loureiro, S.M.A. Pinto, J. Pina, C. Serpa, "Interaction Between a Water-soluble Anionic Porphyrin and Human Serum Albumin Unexpectedly Stimulates the Aggregation of the Photosensitizer at the Surface of the Albumin". *Int. J. Biol. Macromol.*, 255 (2024) 128210.
DOI: 10.1016/j.ijbiomac.2023.128210
82. Sophie Maguire, Grant Strachan, Karolis Norvaiša, Claire Donohoe, Lígia C. Gomes-da-Silva, Mathias O. Senge "Porphyrin Atropisomerism as a Molecular Engineering Tool in Medicinal Chemistry, Molecular Recognition, Supramolecular Assembly, and Catalysis". *Chemistry – A European Journal*, May 2024, e202401559.
DOI.org/10.1002/chem.202401559
83. B.F.A. Pinheiro, N.C. Fernandes, O.A. Chaves, J.A. Ellena, M.S. de Queiroz, A.C. Tedesco, J.H. de Araujo-Neto, S. Nikolaou. "Water-Soluble μ -oxo triruthenium Compound of Biological Interest: H-Bonds Network and Interaction with HSA". *Eur. J. Inorg. Chem.*, 27 (2024) e202300617.
DOI: 10.1002/ejic.202300617
84. B.M. Rodrigues, D.F. de Oliveira, R.Q. Garcia, O.A. Chaves, G.F. Pizzi, L.A.S. Costa, L. de Boni, B.A. Iglesias. "The Photophysical, Photobiological, and DNA/HSA-Binding Properties of Corroles Containing Carbazole and Phenothiazine Moieties". *Int. J. Biol. Macromol.*, 268 (2024) 131861.
DOI: 10.1016/j.ijbiomac.2024.131861
85. F.M. Martins, B.A. Iglesias, O.A. Chaves, J.L.G. da Silva, D.B.R. Leal, D.F. Back. "Vanadium(v) Complexes Derived from Triphenylphosphonium and Hydrazides: Cytotoxicity Evaluation and Interaction with Biomolecules". *Dalton Trans.*, 53 (2024) 8315-8327
DOI: 10.1039/D4DT00464G
86. G.F. Rio, L.H.E. Castro, G.S.R. Souza, O.A. Chaves, M.E.F. de Lima, D. Cesarin-Sobrinho, C.M.R. Sant'Anna. "Evaluation of the Interaction Between New Trypanocide 1,2,4-Triazol-3-Thiones with Human Serum Albumin". *J. Mol. Liq.*, 407 (2024) 125247.

DOI: 10.1016/j.molliq.2024.125247

87. L.B. Trentin, A.R. Viana, S. Iwersen, B.A. Iglesias, O.A. Chaves, A.P. Schuch. "Light Exposure of Tetra-Cationic Porphyrins Containing Peripheral Pd(II)-Bipyridyl Complexes And The Induced Effects on Purified DNA Molecule, Fibroblast and Melanoma Cell Lines". *Photochem. Photobiol.* (2024)

DOI: 10.1111/php.14017

88. F.M. Martins, D.C. Durigon, O.A. Chaves, R.A. Peralta, D.F. Back, H. Terenzi. "Zwitterionic Dioxidovanadium(V) Complexes Containing Fluorinated Triphenylphosphonium Ligands: Structure and Biomacromolecule Studies". *New J. Chem.* 48 (2024) 17722-17733.

DOI: 10.1039/D4NJ03087G

89. R.C. Duarte, R. Cercená, B.B. de Araujo, O.A. Chaves, P.F.B. Gonçalves, E. Zapp, F.S. Santos, F.S. Rodembusch, A.G. Dal-Bó. "Synthesis, Characterization, and BSA Binding Properties of Carboxylated Merocyanine-Based Fluorophores". *ACS Omega* 49 (2024) 48697-48710.

DOI: 10.1021/acsomega.4c07997

90. O.A. Chaves, C.H.C.S. Oliveira, R.C. Ferreira, D. Cesarin-Sobrinho, A.E.H. Machado, J.C. Netto-Ferreira. "Synthetic Dimethoxyxanthenes Bind Similarly to Human Serum Albumin Compared With Highly Oxygenated Xanthenes". *Chem. Phys. Imp.* 8 (2024) 100411.

DOI: 10.1016/j.chphi.2023.100411

91. Zomorodbakhsh, S., Gonzalez, A.C.S., Cruz, I.G., Piccirillo, G., Maria, T.M.R., Marques, I.S., Peixoto, A.F., Gil, J.M., Ferreira, F., Carrilho, R.M.B., *Modified Biochar Materials from Eucalyptus globulus Wood as Efficient CO₂ Adsorbents and Recyclable Catalysts*, *Adv. Sustain. Syst.*, Art. N. 2400431, 2024.

DOI: 10.1002/adsu.202400431

92. Jenei, L.B., Mikle, G., Carrilho, R.M.B., Pereira, M.M., Kollár, L., *Synthesis of p-phenylene-based chiral dicarboxamides via aminocarbonylation of 1',4'-diiodostyrene*, *Tetrahedron*, 2024, 160, 134049

DOI: 10.1016/j.tet.2024.134049.

93. Fonseca, I.C.F., Pais, M.L., Rodrigues, F.M.S., Sereno, J., Castelo-Branco, M., Cavadas, C., Pereira, M.M., Abrunhosa, A.J., *Improved Chemical and Radiochemical Synthesis of Neuropeptide Y Y2 Receptor Antagonist N-Methyl-JNJ-31020028 and Preclinical Positron Emission Tomography Studies*, *Pharmaceuticals*, 2024, 17, 474

DOI: 10.3390/ph17040474

94. Marques, D.L., Piccirillo, G., Rodrigues, F.M.S., Aroso, R.T., Dias, L.D., da Silva, G.J., Calvete, M.J.F., Pereira, M.M. *Advancing Continuous Flow Techniques for Effective Trimethoprim Oxidation: Combatting Bacterial Resistance in Wastewater*, *ChemComm*, 2024

DOI: 10.1039/D4CC04504A

95. Piccirillo, G., Aroso, R.T., Baptista, J.A., Castro, R.A. E., da Silva, G.J., Calvete, M.J.F., Pereira, M.M., Canotilho, J., Eusébio, M.E.S. *Trimethoprim-Based Multicomponent Solid Forms: Mechanochemical Screening, Characterization and Antibacterial Activity Assessment*, *Int. J. Pharmaceutics*, 2024, 661, 124416

DOI: 10.1016/j.ijpharm.2024.124416

96. Rodrigues, F.M.S., Masliy, V., Hryhoryev, Y., Dias, L.D., Carrilho, R.M.B., Calvete, M.J.F., Takács, A., Mikle, G., Kollár, L., Pereira, M.M., *Gas-Liquid Tubular Continuous-Flow Pd-catalysed Aminocarbonylation Process for Scalable Synthesis of Carboxamides*, *Catal. Sci. Technol.*, 2024, 14, 4245-4255.

DOI: 10.1039/D4CY00633J

97. Maldonado-Carmona, N., Piccirillo, G., Godard, J., Heuzé, K., Genin, E., Villandier, N., Calvete, M.J.F., Leroy-Lhez, S. *Bio-based matrix photocatalysts for photodegradation of antibiotics*, *Photochem. Photobiol. Sci.*, 2024, 23, 587-627.

DOI: 10.1007/s43630-024-00536-3

98. Nobre, L.C. S., Teixeira, P., Pinheiro, C.I.C., Palavra, A.M.F., Calvete, M.J.F., de Castro, C.A.N., Nobre, B.P. *The Treatment of Natural Calcium Materials Using the Supercritical Antisolvent Method for CO₂ Capture Applications*, *Processes*, 2024, 12, 425.

DOI: 10.3390/pr12030425

99. Carrilho, R.M.B., Calvete, M.J.F., Mikle, G., Kollár, L., Pereira, M.M., *Carbon monoxide as a C1 building block in fine chemical synthesis*, Chinese Journal of Chemistry, 2024, 42, 199-221. DOI: 10.1002/cjoc.202300384

100. Roque, J. P. L., Nunes, C. M., Saito, F., Bernhardt, B., Fausto, R., Schreiner, P. R., *Competitive Heavy-Atom Tunneling Reactions Controlled Through Electronic Effects*, ChemistryEurope 2024, e202400060. DOI: 10.1002/ceur.202400060

101. Jesus, A. J. L., Nunes, C. M., Ferreira, G. A., Keyvan, K., Fausto, R., *Photochemical Generation and Characterization of C-Aminophenyl-Nitrilimines: Insights on Their Bond-Shift Isomers by Matrix-Isolation IR Spectroscopy and Density Functional Theory Calculations*, Molecules 2024, 29, 3497. DOI: 10.3390/molecules29153497

102. Roque, J. P. L., Nunes, C. M., Schreiner, P. R., Fausto, R., *Hydrogen Tunneling Exhibiting Unexpectedly Small Primary Kinetic Isotope Effects*, Eur. Chem. J. 2024, 30, e202301103. DOI: 10.1002/chem.202401323

103. Nunes, C. M., Roque, J. P. L., Rosado, M. T. S., Fausto, R., *On the Carbenic Nature of Nitrile Ylides: Experimental and Computational Characterization of Hydroxy and Amino Nitrile Ylides*, Eur. J. Org. Chem. 2024, 27, e202301103. DOI: 10.1002/ejoc.202301103

104. Jaleh, B., Kashfi, M., Mohazzab, B. F., Niaee, M. S., Vafaei, F., Fakhri, P., Golbedaghi, R., Fausto, R., *Experimental Characterization and Finite Element Investigation of SiO₂ Nanoparticles Reinforced Dental Resin Composite*, Sci. Reports. – Nature, 2024, 14, 7794. DOI: 10.1038/s41598-024-58114-7

105. Nogueira, B. A., Lopes, S. M. M., Rodrigues, A. C. B., Eusébio, M. E. S., André, V., Duarte, T., Paixão, J. A., Pinho e Melo, T. M. V. D. Fausto, R., *Unveiling the Red and Brownish-Green Polymorphs of a Novel ROY Derivative: 2-(4-((3-Cyanothiophen-2-yl)amino)-3-nitrophenyl)acetic acid*, Cryst. Growth Des. 2024, 24, 947. DOI: 10.1021/acs.cgd.3c00941

106. Gomes, C., Costa, M., Lopes, S. M. M., Nogueira, B. A., Fausto, R., Paixão, J. A., Pinho e Melo, T. M. V. D., Martins, L. M. D. R. S., Pineiro, M., *On the Mechanochemical Synthesis of C-Scorpionates with Oxime Moiety and Their Application in the CuAAC Reaction*, New J. Chem. 2024, 48, 874. DOI: 10.1039/D3NJ05017C

107. Sequeira, M. C. M., Nogueira, B. A., Caetano, F. J. P., Diogo, H. P., Fareleira, J. M. N. A., Fausto, R., *Di-Alkyl Adipates as New Phase Change Material for Low Temperature Energy Storage*, Intl. J. Thermophys. 2023, 44, 165. Correction: ibidem, 2024, 45, 2. DOI: 10.1007/s10765-023-03301-3

108. Sanati, A. L., Nikitin, T., Fausto, R., Majidi, C., Tavakoli, M., *Graphene-Assisted Chemical Stabilization of Liquid Metal Nano Droplets for Liquid Metal Based Energy Storage*, J. Adv. Mater. Tech. 2024, 2301428. DOI: 10.1002/admt.202301428

109. Brás, E. M., Zimmermann, C., Fausto, R., Suhm, M. A., *Benchmarking the Anisotropy of Nitroxyl Radical Solvation with IR Spectroscopy*, Phys. Chem. Chem. Phys. 2024, 26, 5822. DOI: 10.1039/D3CP05668F

110. Sequeira, M. C. M., Nogueira, B. A., Caetano, F. J. P., Diogo, H. P., Fareleira, J. M. N. A., Fausto, R., *Solid-liquid Phase Equilibrium: Alkane Systems for Low Temperature Energy Storage*, Intl. J. Thermophys. 45 (2024) 1. DOI: 10.1007/s10765-023-03317-9

111. Secrieru, A., Lopes, S., Nikitin, T., Cristiano, M. L. S., Fausto, R., *4-Hydroxyquinolin-2(1H)-one Isolated in Cryogenic Argon and Xenon Matrices: Tautomers and Photochemistry*, J. Mol. Struct. 2024, 1312, 138412. DOI: 10.1016/j.molstruc.2024.138412

112. Góbi, S., Reva, I., Ragupathy, G., Fausto, R., Tarczay, G., *Hydrogen-atom-assisted Tautomerization on Solid Surfaces – The Case Study of Thioacetamide*, J. Phys. Chem. C 2024, 128, 21691.
DOI: 10.1021/acs.jpcc.4c05817
113. Talebi, A., Saleh, M., Lopes Jesus, A. J., Kubicki, M., Fausto, R., Golbedaghi, R., *New Azide-Bridged Polymeric Manganese (III) Schiff Base Complex with Allylamine-Derived Ligand: Structural Characterization, Activity Spectra and Molecular Docking*, Inorganics 2024, 12, 234.
DOI: 10.3390/inorganics12090234
114. Ghasemlou, S., Li, X., Galimberti, D., Nikitin, T., Fausto, R., Xue, J., Holleman, S., Rasing, T., Cuppen, H. M., *Identifying and controlling the Order Parameter for Ultrafast Photoinduced Phase Transitions in Thermosensitive Materials*, PNAS 2024, 121, e2408366121.
DOI: 10.1073/pnas.2408366121
115. Dogam, G. Y., Halimoglu, G., Kapanoglu, D., M. Aksoy, U., Kandeger, A., Yavuz, E., Kartal, S., Fausto, R., Ildiz, G. O., *Raman Spectra of Blood Serum as a Holistic Biomarker for Differential Auxiliary Diagnosis of Attention Deficit and Hyperactivity Disorder (ADHD) in Adults*, Spectrosc. J. 2024, 2, 53.
DOI: 10.3390/spectroscj2020004
116. Braz, S., Justino, L. L. G., Ramos, M. L., Fausto, R., *Indigo Carmine Binding to Cu(II) in Aqueous Solution and Solid State: Full Structural Characterization Using NMR, FTIR and UV/Vis Spectroscopies and DFT Calculations*, Molecules, 2024, 29, 3223.
DOI: 10.3390/molecules29133223
117. Nogueira, B. A., Fausto, R., *The ROY Family's Growing Palette: Insights into Recent Compound Additions and Color Range Expansion - A Short Review*, J. Mol. Struct. 2024, 1318, 139220.
DOI: 10.1016/j.molstruc.2024.139220
118. M. C. M. Sequeira, T. Nikitin, F. J. P. Caetano, H. P. Diogo, J. M. N. A. Fareleira and R. Fausto, *Solid-Liquid Phase Equilibrium of the n-nonane + n-undecane System for Low-Temperature Thermal Energy Storage*, Intl. J. Thermophys. 2024, 10765, 3411.
DOI: 10.1007/s10765-024-03411-6
119. Fausto, R., Ildiz, G. O., Nogueira, B.A., *Revisiting Structural, Vibrational and Photochemical Data of Matrix-Isolated Simple Hydantoins – Common Features and Substituents Effects*, Low Temp. Phys. 2024, 50, 785.
DOI: 10.1063/10.0028129
120. Ghoudi, A., Chaabane, I., Aydi, A., Dhahri, A., Costa, B. F. O., Nikitin, T., Paixão, J. A., Fausto, R., *Optical and Electric Properties of the Organic-Inorganic Hybrid bis(2-Amino-5-picolinium) Tetrachlorocobaltate(II) [(C₆H₇N₂)₂CoCl₄]*, Inorg. Chem. Commun. 2024, 168, 112925.
DOI: 10.1016/j.inoche.2024.112925
121. Sıdır, İ., Lopes, S., Nikitin, T., Sıdır, Y. G., Fausto, R., *Infrared Spectroscopy and Photochemistry of Ethyl Maltol in Low-Temperature Ar Matrix*, Spectrosc. J. 2024, 2, 188.
DOI: 10.3390/spectroscj2040013
122. Baptista, J., Castro, R. A. E., Fantechi, E., Chelazzi, L., Ciattini, S., Rosado, M. T. S., Eusébio, M. E. S., *Prolific solid-form landscape of probucol: crystallization from solutions*, Cryst. Growth Des., 2024.
DOI: 10.1021/acs.cgd.4c01603
123. Silva, J. F. C., Jasiurkowska-Delaporte, M., Silva, P. S. P., Silva, M. R., Eusébio, M. E. S., Rosado, M. T. S., *Avoiding pits on the energy landscape – alternative strategies for stabilizing nateglinide co-amorphous systems*, CrystEngComm. 26, 3653, 2024.
DOI: 10.1039/D4CE00195H
124. Almeida, A. C., Ferreira, P. O., Porto, M. V., Canotilho, J., Castro, R. A. E., Caires, F. J., Eusébio, M. E. S., *Novel nimesulide multicomponent solid forms: screening, synthesis, thermoanalytical study and characterization*, J. Therm. Anal. Calorim., 2024.
DOI: 10.1007/s10973-024-13189-2

125. Zomorodbakhsh, S., Gonzalez, A. C. S., Cruz, I. G., Piccirillo, G., Maria, T. M. R., Marques, I. S., Peixoto, A. F., Gil, J. M., Ferreira, F., Carrilho, R. M. B., *Modified Biochar Materials from Eucalyptus globulus Wood as Efficient CO₂ Adsorbents and Recyclable Catalysts*, *Adv. Sustain. Syst.*, 400431, 2024.
DOI: 10.1002/adsu.202400431
126. Nunes, C. M., Lopes Jesus, A. J., Rosado, M. T., S., Fausto, R., *On the Carbenic Nature of Nitrile Ylides: Experimental and Computational Characterization of Hydroxy and Amino Nitrile Ylides*, *EurJOC*, 23, e202301103, 2024.
DOI: 10.1002/ejoc.202301103
127. Brito, A. L. B., Cardoso, I. F., Viegas, L. P., Fausto, R., *Semi-quantitative chemometric models for characterization of mixtures of sugars using infrared spectral data*, *Spectrochim. Acta A*, 326, 125225 (2024).
DOI: 10.1016/j.saa.2024.125225
128. Viegas, L. P., Galvão, B. R. L., *With a little help from our (Al) friend: A general transition state sampling method for tropospheric hydrogen abstraction reactions*, *Atmos. Environ.*, 328, 120515 (2024).
DOI: 10.1016/j.atmosenv.2024.120515
129. Varandas, A. J. C., *C_n, C_nH and their anions: Quest for linearity with n ≤ 8 even versus odd, and beyond*, *Int. J. Quantum Chem.*, 124, e27287 (2024).
DOI: 10.1002/qua.27287
130. Varandas, A. J. C., *Boron and nitrogen cluster families analogous to carbon family: how quasi-molecule theory predicts their planarity or otherwise*, *Mol. Phys.* (2024)
DOI: 10.1080/00268976.2024.2334808
131. Varandas, A. J. C., *Tipping point to explain melamine's non-planarity or otherwise. Can quasi-molecules be "seen" in the parent molecule?*, *Chem. Phys. Lett.*, 852, 141493 (2024).
132. Mondal, T., Varandas, A. J. C., *On the rearrangement and dissociation mechanism of SiH⁴⁺ in its triply-degenerate ground state*, *J. Chem. Phys.*, 160, 234302 (2024).
DOI: 10.1063/5.0213425
133. Guan, Y. F., Chen, Q., Varandas, A. J. C., *Accurate diabaticization based on combined-hyperbolic-inverse-power-representation: 1,2 2A states of BeH²⁺*, *J. Chem. Phys.*, 160, 154105 (2024).
DOI: 10.1063/5.0200732
134. Hazra, S., Naskar, K., Adhikari, S., Varandas, A. J. C., *Ortho-Para Conversion for H⁺ + H₂ Collision in Low Temperature: A Fully Close-Coupled Time-Dependent Wave Packet Study*, *J. Chem. Phys.*, 128, 8833 (2024).
DOI: 10.1021/acs.jpca.4c02243
135. Freitas, D. P., Pansini, F. N. N., Varandas, A. J. C., *Optimized infrared spectrum of (H₂O)_m:(HCN)_n mixtures*, *J. Comp. Chem.*, 45, 2842.
DOI 10.1002/jcc.27491
136. Lu, D. D., Galvao, B. R. L., Varandas, A. J. C., Guo, H., *Quantum and semiclassical studies of nonadiabatic electronic transitions between N(4S) and N(2D) by collisions with N₂*, *Phys. Chem. Chem. Phys.*, 26, 12893
DOI: 10.1039/d4cp90064b
137. Tak, A., Srikanth, K., Kumar, A., Koner, D., González-Lezana, T., Varandas, A. J. C., Rao, T. R., *Theoretical study of S plus SH reaction on its ground state HS₂(X 2A⁺) potential energy surface*, *Mol. Phys.*, Mol Phys. (in press, 2024).
DOI: 10.1080/00268976.2024.2362385
138. Fiorini, L., Morais, W. P., Batista, N. N., de Souza, F. A. L., Varandas, A. J. C., Paz, W. S., Pansini, F. N. N., *Hydrogen-designed spin-states of 2D silicon carbide and graphene nanostructures*, *Phys. Chem. Chem. Phys.*, 26, 26576 (2024).
DOI: 10.1039/d4cp02762k

139. Sousa, S., Vasconcelos, V., Caridade, P. J. S. B., *Evaluating the Impact of Filtering Techniques on Deep Learning-Based Brain Tumour Segmentation*, *Computers*, 13, 237 (2024).
DOI: 10.3390/computers13090237

140. Hendrikx, M. M., Pereira, A. M. R., Pereira, A. B., Carvalho, C. S. C., João L. P. Ribeiro, J. L. P., Soares, M. I. L., Saraiva,* L., Pinho e Melo, *T. M. V. D., *Chiral Hydroxymethyl-1H,3H-pyrrolo[1,2-c]thiazoles: the Search for Selective p53-Activating Agents for Colorectal Cancer Therapy*, *RSC Med. Chem.*, 15, 1652-1663, 2024.
DOI: 10.1039/d4md00076e

141. Cardoso, M., Marto, C. M., Paula, A., Coelho, A. S., Coelho, A. S., Amaro, I., Pineiro, M., Pinho e Melo, T. M. V. D., Ferreira, M. M., Botelho, M. F., Carrilho, E., Laranjo, M., *Effectiveness of photodynamic therapy on treatment response and survival in patients with recurrent oral squamous cell carcinoma: a systematic review*, *Photodiagnosis and Photodynamic Therapy*, 48, Art. No. 104242, 2024.
DOI: 10.1016/j.pdpdt.2024.104242

142. Grosso, C., Alves, C., Sase, T. J., Alves, N. G., Cardoso, A. L., Lemos, A., Pinho e Melo, T. M. V. D., *Selective Synthesis of 3-(1H-Tetrazol-5-yl)-Indoles from 2H-Azirines and Arynes*, *ACS Omega*, 9, 29282-29289, 2024.
DOI: 10.1021/acsomega.4c00305

143. Ribeiro, J. L. P., Costa, I., Silva, R., Lopes, S. M. M., Saraiva, L., Pinho e Melo, T. M. V. D., *3-Tetrazolyl- β -carboline Derivatives as Potential Neuroprotective Agents*, *Bioorg. & Med. Chem.*, 111, Art. No. 117841, 2024.
DOI: 10.1016/j.bmc.2024.117841

144. Alves, A. J. S., Silvestre, J. A. D., Pinho e Melo, T. M. V. D., *Continuous Flow Spirocyclization Reactions: Towards Efficient Synthesis of Chiral Spiropenicillanates*, *Eur. J. Org. Chem.*, 27, Art. No. e202400689, 2024.
DOI: 10.1002/ejoc.202400689

145. Carvalho, C., Silva, R., Pinho e Melo, T. M. V. D., Inga, A., Saraiva, L., *p53 and the ultraviolet radiation-induced skin response: finding the light in the darkness of triggered carcinogenesis*, *Cancers*, 16, Art. No. 3978, 2024.
DOI: 10.3390/cancers16233978

146. Amorim, A. C., Burke, A. J., *What is the future of click chemistry in drug discovery and development?*, *Expert Opinion on Drug Discovery (EODC)*, 19, 267-280, 2024.
DOI: 10.1080/17460441.2024.2302151

147. Moutayakine, A., Burke, A. J., *Sequential Chan-Lam Coupling/Carbonylative Cyclization versus Buchwald-Hartwig Coupling/Carbonylative Cyclization for accessing Dibenzodiazepinones*, *Beilstein J. Org. Chem.*, 20, 193-204, 2024.
DOI: 10.3762/bjoc.20.19

148. Puerta, A., González-Bakker, A., Brandão, P., Pineiro, M., Burke, A. J., Giovannetti, E., Fernandes, M. X., Padrón, J. M., *Early pharmacological profiling of isatin derivatives as potent and selective cytotoxic agents*, *Biochemical Pharmacology*, 222, Art. No. 116059, 2024.
DOI: 10.1016/j.bcp.2024.116059

149. Carreiro, E. P., Hermann, G. J., Federsel, H.-J., Burke, A. J., *Asymmetric Catalytic Synthesis of APIs in Deep Eutectic Solvents: A survey across the catalytic spectrum*, *Catalysts*, 14, Art. No. 160, 2024.
DOI: 10.20944/preprints202401.1254.v1

150. Carreiro, E. P., Hermann, G. J., Federsel, H.-J., Burke, A. J., *Asymmetric Additions Empowered by OrganoCatalysts, Metal Catalysts, and Deep Eutectic Solvents (NADES)*, *J. Org. Chem.*, 89, 10, 6631–6638, 2024.
DOI: 10.1021/acs.joc.4c00334

151. Gastalho, C. M., Sena, A. M., López, Ó., García-Sosa, A. T., Antunes, C. M., Costa, A. R., Burke, A. J., Carreiro, E. P., *Assessing the Potential of 1,2,3-Triazole-Dihydropyrimidinone Hybrids against Cholinesterases: In Silico, In Vitro and In Vivo studies*, *Int. J. Mol. Sci.*, 25(20), Art. No. 11153, 2024.
DOI: 10.3390/ijms252011153
152. Teixeira, C., Gomes, S., Burke, A. J., *Revisiting the Algar-Flynn-Oyamada Reaction Mechanism: Insights from Computational and Synthetic Experiments*, *Beilstein J. Org. Chem.*, 2024, Art. No. 202427.
DOI: 10.3762/bxiv.2024.27.v1
153. Almeida, Z. L., Vaz, D. C., Brito, R. M. M., *Transthyretin mutagenesis: impact on amyloidogenesis and disease*. *Crit. Rev. Clin. Lab. Sci.*, 61, 616–640, 2024.
DOI: 10.1080/10408363.2024.2350379
154. Amado, D., Chaves, O. A., Cruz, P. F., Loureiro, R. J. S., Almeida, Z. L., Jesus, C. S. H., Serpa, C., Brito, R. M. M., *Folding Kinetics and Volume Variation of the β -Hairpin Peptide Chignolin upon Ultrafast pH-Jumps*. *J. Phys. Chem. B*, 128, 4898–4910, 2024.
DOI: 10.1021/acs.jpcc.3c08271
155. Cardoso, R.M.S., Lairion, F., Disalvo, E.A., Loura, L.M.S., Moreno, M.J. *Dipole Potential of Monolayers with Biologically Relevant Lipid Compositions*, *Molecules*, 29, Art. N. 5843, 2024.
DOI: 10.3390/molecules29245843.
156. Chaves, O. A., Loureiro, R. J. S., Serpa, C., Cruz, P. F., Ferreira, A. B. B., Netto-Ferreira, J. C., *Increasing the polarity of β -lapachone does not affect its binding capacity with bovine plasma protein*. *Int. J. Biol. Macromol.*, 263, Art. N. 130279, 2024.
DOI: 10.1016/j.ijbiomac.2024.130279
157. Correia, I., Antunes, M., Tecelão, C., Neves, M., Pires, C. L., Cruz, P. F., Rodrigues, M., Peralta, C. C., Pereira, C. D., Reboredo, F., Moreno, M. J., Brito, R. M. M., Ribeiro, V. S., Vaz, D. C., Campos, M. J., *Nutritive Value and Bioactivities of a Halophyte Edible Plant: *Crithmum maritimum* L. (Sea Fennel)*, *Plants*, 13, Art. N. 427, 2024.
DOI: 10.3390/plants13030427
158. Galdes, C.F.G.C., *Rational Design of Magnetic Nanoparticles as T1-T2 Dual Mode MRI Contrast Agents*, *Molecules*, 29, Art. N. 1352, 2024.
DOI: 10.3390/molecules29061352
159. Gigli, L., Silva, J. M., Cerofolini, L., Macedo, A. L., Galdes, C.F.G.C., Suturina, E.A., Calderone, V., Fragai, M., Parigi, G., Ravera, E., Luchinat, C., *Machine Learning-Enhanced Quantum Chemistry-Assisted Refinement of the Active Site Structure of Metalloproteins*, *Inorg. Chem.*, 63, 10713–10725, 2024.
DOI: 10.1021/acs.inorgchem.4c01274
160. Griffith, M., Araújo, A., Travasso, R., Salvador, A., *The architecture of redox microdomains: Cascading gradients and peroxiredoxins' redox-oligomeric coupling integrate redox signaling and antioxidant protection*, *Redox Biol.*, 69, Art. N. 103000, 2024.
DOI: 10.1016/j.redox.2023.103000
161. Karagöz, M. F., Koçyiğit, E., Koçak, T., Özturan Şirin, A., Icer, M. A., Ağagündüz, D., Coreta-Gomes, F., *Decoding coffee cardiometabolic potential: Chemical composition, nutritional, and health relationships*. *Compr. Rev. Food Sci. Food Saf.*, 23, Art. N. e13414, 2024.
DOI: 10.1111/1541-4337.13414
162. Machado, F., Coimbra, M. A., Castillo, M. D. del, Coreta-Gomes, F., *Mechanisms of action of coffee bioactive compounds – a key to unveil the coffee paradox*, *Crit. Rev. Food Sci. Nutr.*, 64, 10164–10186, 2024.
DOI: 10.1080/10408398.2023.2221734
163. Machado, F., Gómez-Domínguez, I., Hurtado-Ribeira, R., Martín, D., Coimbra, M. A., Castillo, M. D. del, Coreta-Gomes, F., *In vitro human colonic fermentation of coffee arabinogalactan and melanoidin-rich fractions*. *Int. J. Biol. Macromol.*, 275, Art. N. 133740, 2024.
DOI: 10.1016/j.ijbiomac.2024.133740

164. Magalhães, S., Aliaño-González, M. J., Cruz, P. F., Rosenberg, R., Haffke, D., Norgren, M., Alves, L., Medronho, B., da Graça Rasteiro, M., *Customising Sustainable Bio-Based Polyelectrolytes: Introduction of Charged and Hydrophobic Groups in Cellulose*, *Polymers*, 16, 3105, 2024.
DOI: 10.3390/POLYMI16223105

165. Morán-Lalangui, M., Coutinho, A., Prieto, M., Fedorov, A., Pérez-Gil, J., Loura, L.M.S., García-Álvarez, B. *Exploring protein-protein interactions and oligomerization state of pulmonary surfactant protein C (SP-C) through FRET and fluorescence self-quenching*, *Protein Sci.*, 33, Art. N. e4835, 2024.
DOI: 10.1002/pro.4835

166. Oliveira, A.C., Filipe, H.A.L., Geraldes, C.F.G.C., Voth, G.A., Moreno, M.J., Loura, L.M.S., *Interaction of MRI Contrast Agent [Gd(DOTA)]⁻ with Lipid Membranes: A Molecular Dynamics Study*, *Inorg. Chem.* 63, 10897-10914, 2024.
DOI: 10.1021/acs.inorgchem.4c00972

167. Pereira, C. D., Guimarães, C., Ribeiro, V. S., Vaz, D. C., Martins, M. J., *Low-Protein Diets, Malnutrition, and Bone Metabolism in Chronic Kidney Disease*, *Nutrients*, 16, Art. N. 3098, 2024.
DOI: 10.3390/NU16183098

168. Pires, C. L.; Moreno, M. J., *Improving the Accuracy of Permeability Data to Gain Predictive Power: Assessing Sources of Variability in Assays Using Cell Monolayers*, *Membranes*, 14, Art. N. 157, 2024.
DOI:10.3390/membranes14070157

169. Salvador, A., *Pillars of theoretical biology: “Biochemical systems analysis, I, II and III.”* *J. Theor. Biol.* 576, Art. N. 111655, 2024.
DOI: 10.1016/j.jtbi.2023.111655

170. Santos, O., Vaz, D., Sebastião, F., Sousa, H., Vieira, J., *Wastewater as a nutrient source for hydroponic production of lettuce: Summer and winter growth*. *Agric. Water Manage.*, Art. N. 301, 108966, 2024.
DOI: 10.1016/J.AGWAT.2024.108966

171. Sebastião, F., Vaz, D. C., Pires, C. L., Cruz, P. F., Moreno, M. J., Brito, R. M. M., Cotrim, L., Oliveira, N., Costa, A., Fonseca, A., Rodrigues, M., Ispolnov, K., Bernardino, R., Vieira, J., *Nutrient-efficient catfish-based aquaponics for producing lamb’s lettuce at two light intensities*. *J. Sci. Food Agric.*, 104, 6541–6552, 2024.
DOI: 10.1002/jsfa.13478

172. Silva, S. P., Coreta-Gomes, F., Coimbra, M. A., Coelho, E., *Pine nut skin as a source of phytosterols and alkanediols - Hypocholesterolemic potential and development of sustainable vegan emulsifiers*, *LWT*, 197, Art. N. 115934, 2024.
DOI: 10.1016/j.lwt.2024.115934

173. Varandas, P.A.M.M., Belinha, R., Cobb, A.J.A., Prates Ramalho, J.P., Segundo, M.A., Loura, L.M.S., Silva, E.M.P., *Flow-based bioconjugation of coumarin phosphatidylethanolamine probes: Optimised synthesis and membrane molecular dynamics studies*, *Biochim. Biophys. Acta. Biomembr.* 1866, Art. N. 184335, 2024.
DOI: 10.1016/j.bbamem.2024.184335

174. Vaz, D. C., Rodrigues, J. R., Loureiro-Ferreira, N., Müller, T. D., Sebald, W., Redfield, C., Brito, R. M. M., *Lessons on protein structure from interleukin-4: All disulfides are not created equal*. *Proteins: Struct., Funct., Bioinf.*, 92, 219–235, 2024.
DOI: 10.1002/PROT.26611

175. Zou, J., Yu, Z., He, F., Luo, S., Ke, L., Gu, H., Coreta-Gomes, F., Wall, P., *Spatial distribution of antioxidant activity in baguette and its modulation of proinflammatory cytokines in RAW264.7 macrophages*, *Npj Sci. Food*, 8(1), Art. N. 63, 2024.
DOI: 10.1038/s41538-024-00302-w

Articles in National Peer-Reviewed Journals (4)

1. Dias, C. M. F., Sobral, A. J. F. N., Gil, J. M., *Armazenamento de Hidrogénio em Materiais Porosos da Classe MOF (Metal-Organic Framework)*, H2 Magazine da Associação Portuguesa para a Promoção do Hidrogénio, nº13, Março-Abril, 38-41, 2024.

2. L.G.A. do Nascimento, M.F.S. Barbeta, O.A. Chaves, A.R.M. de Oliveira, S. Nikolaou. “Interaction of a Triruthenium ortho-Metallated Phenazine with Cytochrome P450 Enzymes”. J. Braz. Chem. Soc. 35 (2024) e-20240136.

DOI: 10.21577/0103-5053.20240136

3. Nogueira, B. A., Fausto, R., *Camaleões Moleculares – Desenvolvimento e Caracterização de Moléculas que Mudam de Cor*, Bol. Soc. Port. Quím. 2024, 48, 53.

DOI: 10.52590/M3.P709.A30002771

4. Marques, A. P. S., Oliveira, R., Ramos, A., Håkonsen, V., Pereira, L. F. R., Murtinho, D. M. B., Alves, L. C., Ferreira, P. J. T., Carvalho, M. G. V. S., Gamelas, J. A. F., *Filmes de Celulose Nanofibrilada – Um Novo Método Inovador para a Conservação e o Restauro de Documentos Antigos Contendo Tinta Ferrogálica*, Info@Tecnicepa (Revista da Tecnicepa - Associação Portuguesa dos Técnicos das Indústrias de Celulose e Papel), 74, 30–33, 2024.

Disponível em: <https://www.tecnicepa.com/files/a407an20240514145910.pdf>

Communications at International Meetings (169)

International Keynotes / Plenary / Invited Lectures (39)

1. Valente, A. J. M., *Cyclodextrin-based polymers: synthetic routes and applications*, 6th edition of French Brazilian Meeting on Polymers, Florianópolis, Santa Catarina, Brazil, , 2024. **Invited Lecture.**
2. Valente, A. J. M., *Mesoporous Materials – Synthesis and Applications*, 16th Latin American Conference on Physical Organic Chemistry, Florianópolis, Santa Catarina, Brazil, 2024. **Plenary Lecture.**
3. Campos, M. G., Anjos, O. Bee pollen and bee bread as source of protein and bioactive compounds. UNIFood Conference. 28, 29 June, 2024 University of Belgrade. Serbia **Invited Oral Communication**
- 4.. Luis G. Arnaut “*Tumor Priming and Photodynamic Therapy: A Renewed Hope for Oncology*”. XXXV Annual Conference of the Italian Society for Photobiology, 9-11/09/2024, Messina (Itália). **Invited Lecture**
5. Luis G. Arnaut. “*Flash Photodynamic Therapy*”. 18th International Congress of Photobiology IUPB, 25-30/08/2024, Perth (Austrália). **Invited Lecture**
6. Luis G. Arnaut. “*Photoacoustic Waves as Enablers of Therapies*” 22nd International Conference on Photoacoustic and Photothermal Phenomena, 8-12/07/2024, Coimbra. **Invited Lecture**
7. Luis G. Arnaut. “*Strategies to Improve Cell Uptake of Medicines*”. Chemistry Towards Biology II, 1-4/07/2024, Cracóvia (Polónia). **Invited Lecture**
8. Luis G. Arnaut. “*The Beauty of Simplicity: The Smallest Porphyrin Derivatives for Photodynamic Therapy*”. 13th Conference on Porphyrins and Phthalocyanines, 23-28/06/2024, Niagara Falls & Buffalo (EUA). **Invited Lecture**
9. C. Serpa, J. Santos, D.A. Pereira, C.P. João, L.C. Gomes-da-Silva, L.G. Arnaut, “*Photoacoustics in action*”. 8th JIF Jornadas Ibéricas de Fotoquímica, 1st FICP Franco-Iberian Conference of Photochemistry, Lisbon, Portugal, 11-13, September 2024. **Invited Lecture**
10. Lígia C. Gomes-da-Silva. “*The role of atropisomerism in enhancing amphiphilicity and cellular internalization of photosensitizers*” 18th International Congress on Photobiology, Perth, Australia, 26 to 30 August 2024, **Invited Lecturer**
11. Lígia C. Gomes-da-Silva. “*Mechanisms of cell death induced by photoactivated bacteriochlorins that accumulate at the endoplasmic reticulum and Golgi compartments*”, 18th International Congress on Photobiology, Perth, Australia, 26 to 30 August 2024, **Invited Lecturer**
12. Pereira, M.M., *Química Medicinal na Universidade de Coimbra*, Univ. Evangélica de Goiás, Anápolis, Brasil, 2024.
Plenary Lecture – School Year Opening Ceremony
13. Pereira, M.M., *Synthesis of Porphyrins via Carbonylation Reactions for Medicinal Applications*, Pécs – Hungary, 2024.
Invited lecture
14. Pereira, M. M., Aroso, R. T., Silva, M. F. C., Domingos, C. V., *Synthesis of Porphyrins Through Continuous Flow Processes and Their Structural Effect on the Photoinactivation of bacteria*, International Conference on Porphyrins and Phthalocyanines (ICPP-13), Buffalo, United States of America, 2024. **Invited Oral Communication**
15. Pinto, S.M.A., Teixeira, D.S., Neves, A., Geraldes, C.F.G.C., Tóth, E., Pereira, M.M., *13th International Conference on Porphyrins & Phthalocyanines*, Niagara Falls, USA, 2024. **Invited Oral Communication**

16. Nunes, C. M., *Tunneling Reactions in Triplet PhenylNitrene Derivatives Generated in Cryogenic Matrices*, XX1st International Workshop on Quantum Atomic and Molecular Tunneling Systems, Donostia / San Sebastián, Spain, 2024. **Invited Oral Communication**
17. Nunes, C. M., *Quantum Tunneling Reactions in PhenylNitrene Derivatives Generated in Cryogenic Matrices*, Institute of Chemical Research of Catalonia, Tarragona, Spain, 2024. **Invited Oral Communication**
18. Fausto, R., *Design, Synthesis and Characterization of Novel Materials Exhibiting Color Polymorphism*, 7th Internatiopnal Conference on Smart Materials and Spectroscopy (SMS'2024), Monastir, Tunisia, 2024. **Plenary Lecture**
19. Fausto, R., *Tunneling-Driven and Vibrationally-Induced Chemistries: Last News from Coimbra!*, XVII International Conference on Molecular Spectroscopy ICMS 2024, Wojanów, Poland, 2024. **Plenary Lecture**
20. Fausto, R., *New Avenues for Molecular Architectures' Manipulation and Controlling Chemical Reactivity: Vibrationally Induced and Quantum Mechanical Tunneling Driven Chemistry*, ReMade Seminar 2024 online: <https://remade-project.eu/index.php/event/vibrationally-induced-and-quantum-mechanical-tunneling-driven-chemistry/> **Invited Oral Communication**
21. Eusébio, M. E. S., *Advancing organic solid-state research: a thermodynamics perspective*. 2 International Symposium on Chemical Thermodynamics for Young Researchers (ISCTYR), Laurino, Italy, 2024. **Plenary Lecture**
22. Rosado, M. T. S., Silva, J. F. C., Eusébio, M. E. S., *Understanding intermolecular interactions in multicomponent solid phases with electronic structure calculations*, Multiscale Phenomena in Condensed Matter, MULTIS 2024, Krakow, Poland, 2024. **Invited Lecture**
23. Rosado, M. T. S., *Cocrystals and co-amorphous solid phases of pharmaceutical interest: synthesis and thermal behavior*, Department of Chemistry and Chemical Technologies, Universirty of Calabria, Cosenza, Italy, 2024. **Invited Oral Communication**
24. Rosado, M. T. S., *Investigation of intermolecular hydrogen bonding in multicomponent solid phases*, Department of Chemistry and Chemical Technologies, Universirty of Calabria, Cosenza, Italy, 2024. **Invited Oral Communication**
25. Fausto, R., *Vibrationally-Induced and Tunneling-Driven Chemistry*, Department of Chemistry, Payame Noor University, Tehran, Iran, 2024. **Invited Oral Communication**
26. Varandas, A.J.C., *From Molecules to 2D Molecular Materials: Attitudinal-Green Approach in Quantum Chemistry*, University of Chinese Academy of Sciences, Beijing, China, 2024. **Plenary Lecture**
27. Varandas, A.J.C., *Molecular Potential Energy Surfaces: A Personal View & Recent Developments*, Qufu Normal University, Qufu, 2024. **Invited Lecture**
28. Varandas, A.J.C., *From Molecular Structure to Dynamics: Attitudinal Green Approach*, Quantum Reactive Scattering, Istanbul, Turkey, 2024. **Plenary Lecture**
29. Varandas, A.J.C., *From Molecules to 2D Molecular Materials: Attitudinal-Green Approach in Quantum Chemistry*, Jining University, Jining, China, 2024. **Invited Lecture**
30. Varandas, A.J.C., *Defying the Curse of Size in Molecular Ab Initio Theory: Tiling for Size, Extrapolation for Accuracy*, Universidad de La Habana, La Habana, Cuba, 2024. **Plenary Lecture**
31. Varandas, A.J.C., *Attitudinal Green Approach to Quantum Chemistry: Tiling for Size, Extrapolation for Accuracy*, II Encontro Capixaba de Física/SBF, Vitória, Brazil, 2024. **Plenary Lecture**
32. Varandas, A.J.C., *From Molecules to H-designed 2D Molecular Materials: Attitudinal-Green Computing*, 9ACCAMP, Shenyang, China, 2024. **Plenary Lecture**

CQC – Overall Output Indicators 2024

33. Varandas, A.J.C., *From Molecules to 2D Molecular Materials: Attitudinal-Green Approach*, QuimiCuba, November, La Habana, Cuba, 2024. **Plenary Lecture**
34. Coreta-Gomes, F., *Decoding Coffee Cardiometabolic Potential: Structure-Health Function Relationships*, International Coffee Convention, Mannheim, Alemanha, 17–18/10/2024. **Keynote Lecture**
35. Figueiredo, A.M., *Modulating Protein Stability and Folding Landscapes via Ion-Pair Interactions and Hydration*. Molten Salts and Ionic Liquids Discussion Group Annual Research Meeting, Imperial College London, United Kingdom, 16/12/2024 **Invited lecture** (invited to give the lecture but unable to attend)
36. Geraldes, C. F.G.C., *MRI contrast agents: T_1 versus paraCEST, NMR Relaxometry for biomedicine and advanced materials*, FC-RELAX Workshop, Lisboa, Portugal, 19-20/04/2024, **Invited Lecture**
37. Pinto, S., Teixeira, D., Neves, A., Geraldes, C. F.G.C., Toth, E., Pereira, M., *The Potential of Tetrapyrrolic Macrocycles as a Platform for Medical Imaging – From Mn(II/III) Redox Contrast Agents for MRI to Radiolabeled Contrast Agents for PET*, International Conference on Porphyrins and Phthalocyanines (ICPP-13), 23-28/06/2024, Niagara Falls, USA. **Invited Lecture**
38. Estes, M. A., *Determinación experimental del Número de Transporte de iones en disolución: un parámetro electroquímico útil para estudiar el sistema electrolítico*, VI Congreso Colombiano de Electroquímica, 20-22 Noviembre, Bogotá (Colombia). **Plenary Lecture.**
39. Abreu, P. E., *In the lab with Brillat-Savarin*, X Iberian Meeting on Colloids and Interfaces, Coimbra, 2024. **Invited Lecture**

International Oral Presentations (42)

1. Ribeiro, A. C. F., Fernandes, F. R.L., Valente, A. J. M., *Difusão acoplada de eletrólitos em soluções aquosas através da aplicação de um modelo matemático e físico. Equações de Nernst-Planck*, XXVI Congresso SIBAE, Faculdade de Ciências da Universidade de Lisboa, Lisboa, 2024. **Oral Presentation**

2. Sofio, S. P. C., Caeiro, A., Canhoto, J., Ribeiro, A. C. F., Valente, A. J. M., Cabral, A. M. T. D. P. V. Esteso, M. A., *EIS como Técnica de Ensaios: Investigação de Fenótipos de Toxicidade na Linha Celular BY-2*, XXVI Congresso SIBAE, Faculdade de Ciências da Universidade de Lisboa, Lisboa, 2024. **Oral Presentation**

3. Galindres-Jiménez, D. M., Maldonado, M., Sanabria, E., Valente, A. J. M., Ribeiro, A. C. F., Esteso, M. A., *Coefficientes de diffusion de C-tetra(pentil)resorcin[4]areno sulfonado en disolución acuosa y a 298,15 K*, XXVI Congresso SIBAE, Faculdade de Ciências da Universidade de Lisboa, Lisboa, 2024. **Oral Presentation**

4. Medronho, B., Duarte, H., Romano, A., Aliaño-González, M., Brás, J., Boutoub, O., Gonçalves, S., Costa, A., Magalhães, S., Fernandes, C., Varela, C., Alves, L., Rasteiro, M. G., Antunes, F., Melro, E., Valente, A., Dahlström, C., Eivazi, A., Norgren, M., *On the valorization of agroforestry residues into novel biobased materials*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Oral Presentation**

5. Matias, P. M. C., Nunes, S. C. C., Rodrigues, A. C. B., Murtinho, D., Pais, A.A. C. C., Valente, A. J. M., *Removal of sulfamethazine and tetracycline from water using a triazine porous organic polymer*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal 2024. **Oral Presentation**

6. Almeida, C. M. R., Oliveira, C., Costa, T., Pina, J., Magalhães, J. M. C. S., Barroso, F., Valente, A., J. M., Durães, L., *Paper-supporting ratiometric sensor probes based on lanthanide complexes for biogenic amines detection*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Oral Presentation**

7. Costa, T., Peixoto, M., Pineiro, M., Seixas de Melo, J. S., *Solvent-Driven Self Organization of Meso-Substituted Porphyrins: Fluorescence Lifetime Imaging Microscopy*, RICIX - The 10th Iberian Meeting on Colloids and Interfaces, Coimbra, Portugal, 2024. **Oral Presentation**

8. dos Santos, D. N. S., Naskar, N., Reess, K., Delgado-Pinar, E., Seixas de Melo, J. S., Rueck, A., *Metabolic imaging with FLIM/PLIM indirubin derivatives: an ultrafast window into cellular metabolism and oxygen consumption*, SPIE Photonics West, Moscone Center San Francisco, California, United States, 2024. **Oral Presentation**

9. dos Santos, D. N. S., Naskar, N., Reess, K., Delgado-Pinar, E., Seixas de Melo, J. S., Rueck, A., *Unravelling the Excited State Deactivation Mechanisms of Indirubin and Its Role in Metabolic and Oxygen Imaging in Living Cells*, VIII Jornadas Ibéricas de Fotoquímica & I Franco-Iberian Conference on Photochemistry, Lisboa, Portugal, 2024.

10. Pereira, M. M.; Rodrigues, F. M. S., *Microsolvation of alkali-metal ions with rare-gas atoms: structure and thermodynamics*, 2nd General Meeting of the COSY COST Action, Wroclaw, Poland, 2024. **Invited Oral Communication**

11. Pacheco, D., Patrício T. M. F., Sobral, A., Mota, C., Encarnação, T., *Bridging Nature's Potential: Harnessing Microalgal Biomolecules for Cutting-Edge Tissue Engineering Applications*, Europeu STRIKE training program: Complementary training: "European Public Funding schemes for R&D and Innovation and Technology Transfer", Faenza, Italy, 2024, January 31. **Oral Presentation**

12. Pacheco, D., Lourenço, Santos, B., Freitas, F., Mateus, A., Cruz, P., Mota, C., Patrício T.M.F., Sobral, A., Encarnação, T., *Bioengineering microalgae *Nannochloropsis* sp. culture to enhance cellulose production*, 3rd International Chemistry Conference PolyChemeet, Lisbon, Portugal, 2024, June 18. **Oral Presentation**

13. Pacheco, D., Lourenço, Santos, B., Freitas, F., Mateus, A., Cruz, P., Mota, C., Patrício T.M.F., Sobral, A., Encarnação, T., *Harnessing Microalgal Polymers for Cutting-Edge Tissue Engineering Applications*, 9th International Conference on Bio-based and Biodegradable Polymers, Coimbra, Portugal, 2024, July 24. **Oral Presentation**

14. Braz, Sofia; Justino, Licinia L. G.; Ramos, M. Luísa; Fausto, Rui. "Indigo carmine food dye (E132) binding to Cu(II) in aqueous solution and solid state: a spectroscopic and DFT characterization study". Trabalho apresentado em *10th Iberian Meeting on Colloids and Interfaces*, 2024. **Oral Presentation**
15. Nunes, S. C. C., Mendes, M., Vitorino, C., Cova, T., Pais, A. A. C. C., *Monte Carlo Simulations for Screening and Optimizing Biopolymer-Based Drug Delivery Systems*, BIOPOL- 9th International Conference on Bio-based and Biodegradable Polymers, Coimbra, Portugal, 22-24 July 2024. **Oral Presentation**
16. D. Amado, O.A. Chaves, R. Loureiro, C.S. Jesus, P.F. Cruz, Z.L. Almeida, C. Serpa, R.M.M. Brito, "Unravelling Protein Folding Dynamics with Photoacoustic Calorimetry: From Amino Acid Mixtures to Model Peptides". 22nd International Conference on Photoacoustic and Photothermal Phenomena, Coimbra, Portugal, 8-12 July 2024. **Oral Presentation**
17. F.A. Schaberle, D. Amado, C. Serpa, "Photoacoustic waves in metals: experimental assessment of wave propagation and surface motion". 22nd International Conference on Photoacoustic and Photothermal Phenomena, Coimbra, Portugal, 8-12 July 2024. **Oral Presentation**
18. C.P. João, J. Santos, R. Barreira, P. Nogueira, C. Serpa, L.G. Arnaut, "Generation of high amplitude photoacoustic pulses in different sources configurations". 22nd International Conference on Photoacoustic and Photothermal Phenomena, Coimbra, Portugal, 8-12 July 2024. **Oral Presentation**
19. D. Vella, D.A. Pereira DA, A. Mrzel A, D. Vengust, L.G. Arnaut, C. Serpa, M. Jezeršek "Picosecond excitation and generation of photoacoustic waves in composites of gold nanoparticles decorated graphene". 22nd International Conference on Photoacoustic and Photothermal Phenomena, Coimbra, Portugal, 8-12 July 2024. **Oral Presentation**
20. D.A. Pereira, D. Vella, E. Sletchi, C. Serpa, L.G. Arnaut, "Exploring Piezophotonic Materials for Efficient Gene Transfection". 22nd International Conference on Photoacoustic and Photothermal Phenomena, Coimbra, Portugal, 8-12 July 2024. **Oral Presentation**
21. L.C. Gomes-da-Silva, A.C. Lobo, M.I. Mendes, D.A. Pereira, C. Serpa, L.G. Arnaut, "Photoacoustic imaging and priming of solid tumors". 22nd International Conference on Photoacoustic and Photothermal Phenomena, Coimbra, Portugal, 8-12 July 2024. **Oral Presentation**
22. Lígia C. Gomes-da-Silva "Photoacoustic imaging and priming of solid tumors". International Conference on Photoacoustic and Photothermal Phenomena (ICPPP22), Coimbra, Portugal, 8-12 July 2024. **Oral Presentation**
23. Mafalda Penetra. "Deciphering the Mechanisms Behind LUZ51 Cellular Internalization and Release", XXVIII Encontro Galego Português de Química, Vigo, Spain, 13-15 November 2024. **Oral Presentation**
24. Livia Stenico "Mechanisms of cell death after photodynamic therapy", European Society for Photobiology Junior Online Meeting, 16 May 2024. **Oral Presentation**
25. Mafalda Penetra *Evaluation of the internalization mechanism of LUZ51*, European Society for Photobiology Junior Online Meeting, 16 May 2024. **Oral Presentation**
26. Arnaut, Z. A., Gomes-da-Silva, L. C., Arnaut, L. G., Pereira, M. M., *Why do the best photosensitizers work?*, IUPB-MEPSA, Perth, Australia, 2024. **Oral Presentation.**
27. Arnaut, Z. A., Felgueiras, A. P., Rodrigues, F., Aroso, R. T., Pais, A. A. C. C., Pereira, M. M., *Factorial design for optimization of tetra-substituted meso-aryl porphyrin synthesis through flow chemistry*, XXVIII Encontro Galego-Português de Química, Vigo, Espanha, 2024. **Oral Presentation.**
28. Felgueiras, A. P., Arnaut, Z. A., Rodrigues, F. M. S., de Oliveira, K. T., Calvete, M. J. F., Pereira, M. M., *Synthesis of BODIPY dyes using flow chemical processes*, ISHC2024 – 29th International Society of Heterocyclic Chemistry Congress, Aveiro, Portugal, 2024. **Oral Presentation**

CQC – Overall Output Indicators 2024

29. Felgueiras, A. P., Arnaut, Z. A., Rodrigues, F. M. S., Cebola, J. S. F., de Oliveira, K. T., Calvete, M. J. F., Pereira, M. M., *Improved synthesis of BODIPY dyes: Batch vs continuous flow chemistry*, XXVIII Encontro Galego portugués de Química, Vigo, Spain, 2024. **Oral Presentation**
30. Domingos, C. V., Aroso, R. T., Silva, M. F. C., Maria, T. M. R., da Silva, G. J., Pereira, M. M. *PLA-Curcumin Biopolymers: Shining a Light onto Potential Photodecontaminating Materials*, 35th Annual Conference & Meeting of the AAIC - Constructing a Sustainable Future, Lisbon, Portugal, September 2024. **Oral presentation.**
31. Teixeira, D.S., Pinto, S.M.A., Tóth, E.J., Pereira, M.M., *Synthesis of tetrapyrrolic macrocycles as potential probes for magnetic resonance imaging*, 29th International Society of Heterocyclic Chemistry Congress, Aveiro, 2024. **Oral Presentation**
32. Anita S. Amorim, Zoe A. Arnaut, Mariette M. Pereira, James P. O`Gara, Luís G. Arnaut, “Use of a small cationic chlorin for antimicrobial Photodynamic Therapy in clinical isolates from patients with DFUs”. Microbiology Annual Meeting, Athlone, Ireland, 06 November 2024. **Oral Presentation**
33. Duarte, L. J., Nunes, C. M., Fausto, R., Braga, A. A. C., *Manipulating Chemical Bonds with IR Radiation*, 4th European Symposium in Chemical Bonding, Amsterdam, Netherlands, 2024. **Oral Presentation**
34. Roque, J. P. L., Nunes, C. M., Fausto, R., Schreiner, P. R., *Directing Competitive Heavy-atom Tunneling Reactions Through Electronic Effects*, XXIst International Workshop on Quantum Atomic and Molecular Tunneling Systems, Donostia / San Sebastián, Spain, 2024. **Oral Presentation**
35. Silva, J. F. C., Eusébio, M. E. S., Rosado, M. T. S., *Going down the thermodynamic stairway from the amorphous phases to the most stable solid forms*, 2 International Symposium on Chemical Thermodynamics for Young Researchers (ISCTYR), Laurino, Italy, 2024. **Oral Presentation**
36. Baptista, J. A., Castro, R. A. E., Fantechi, E., Chelazzi, L., Ciattini, S., Santos, J. C., Marques, J. M. C., Rosado, M. T. S., Eusébio, M. E. S., *New solid-state landscape of an old drug – can structurally related compounds help?*, 2 International Symposium on Chemical Thermodynamics for Young Researchers (ISCTYR), Laurino, Italy, 2024. **Oral Presentation**
37. Rodrigues, S. P. J., Caridade, P. J. S. B., *Computational Chemistry in Graduation Courses of Chemistry*. In 10th International Conference on Higher Education Advances (HEAd'24). Valencia, Spain, 2024. **Oral Presentation**
38. Lopes, S. M. M., Pinho e Melo, T. M. V. D., *Cycloaddition and annulation reactions of steroidal heterodienes*, 29th Congress of the International Society of Heterocyclic Chemistry (ISHC 2024), Aveiro, Portugal, 2024. **Oral Presentation**
39. Machado, T. F., Valente, A. J. M., Silva Serra, M. E., Murtinho, D. *Tröger’s Base–linked POPs as Heterogeneous Catalysts for the Nitroaldol Condensation*, XII Encontro Nacional de Catálise e Materiais Porosos (XII ENCMP), 6–7 junho, Coimbra, Portugal, 2024. **Oral Presentation**
40. Jesus, C. F., Murtinho, D., Alves, A. A. S., Antunes, F. E. *Physico-chemical Characterization of N-alkyldimethylglucosylammonium iodide: new sugar-based cationic surfactants*, X Iberian Meeting on Colloids and Interfaces (RICI X), 23–26 June, Coimbra, Portugal, 2024. **Oral Presentation**
41. Lopes, J., Marques-da-Silva, D., Peralta, C., Rodrigues, J.R., Vaz, D.C., Lagoa, R. *Humic acid aggregates with laccase and decreases the performance of the enzyme catalytic systems through various mechanisms*, 6th International Conference on Green Chemistry and Sustainable Engineering (GreenChem-24), 24-26/07/2024, Lisboa, Portugal. **Oral Presentation**
42. Machado, F., Coimbra, M., Coreta-Gomes, F., *Explore cardioprotective potential of coffee and its extracts*, 4th International Conference on Natural Products and Human Health, Aveiro, Portugal, 18-20/09/2024 (Honorable recognition as best oral presentation). **Oral Presentation**

International Posters (88)

1. Santos, J. A., Murtinho, D., Vitorino, C., Muniz, E. C., Valente, A. J. M., *PVA Hydrogels Loaded with DNA: A Breakthrough in Gene Therapy*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
2. Talles B. Costa, Pedro M.C. Matias, Derval S. Rosa, Dina M.B. Murtinho, A. J. M. Valente, *Removal of potentially toxic metals from aqueous solution using nanocellulose chemically modified by succinylation*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
3. Vareda, J., Sofio, S., Fonseca, A., Pontinha, D., Valente, A. J. M., Ribeiro, A., *Effect of sodium perchlorate on diffusion of poly(vinyl alcohol) in aqueous solutions*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
4. Cabral, A. M. T. D. P. V. D., A. Messias, A., Nicolau, P., Valente, A. J. M., Rodrigo, M., Fernandes, F., Ribeiro, A. C. F., Fangaia, S., *Coupled transport of nickel ions in aqueous electrolytic solutions and surfactants solutions*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
5. Cabral, A. M. T. D. P. V., Ribeiro, A. C. F., Valente, A. J. M., Estesó, M. A., Benavent, A., Rodrigo, M., *Transport Properties of the First-line Antituberculous Drugs in Multicomponent Systems*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
6. Jiménez, D. M. G., Ribeiro, A. C. F., Valente, Estesó, M. A., Vargas, E. F., *Surface tension and aggregation behavior of resorcin[4]arenes in the presence of NaCl and protein*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
7. Sousa, J. F. M., Murtinho, D., Valente, A. J. M., Marques, J. M. C., *Adsorption of tetracycline antibiotic from aqueous solution by chitosan and naphthaldehyde derivatives composites*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
8. Ramos, A. R. A., Matias, P. M. C., Murtinho, D. M. B., Valente, A. J. M., *Synthesis of amine-based cyclodextrin nanosponges for the removal of antibiotics and synthetic dyes*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
9. Machado, T. F., Valente, A. J. M., Silva Serra, E. M., Murtinho, D. M. B., *Diazo- and Tröger's Base-linked POPs for Dye Adsorption from Aqueous Solution*, 10th Iberian Meeting on Colloids and Interfaces - RICIX, Coimbra, Portugal, 2024. **Poster**
10. Ribeiro, A. C. F., Daňková, A. V., Korpasová, K., Musilová, L., Mráček, A., Azevedo, E. F. G., Valente, A. J. M., Estesó, M., *Coupled diffusion of salts and sodium hyaluronate in aqueous solutions*, 9th International Conference on Bio-based and Biodegradable Polymers - BIOPOL, Coimbra, 2024. **Poster**
11. Santos, J. A., Murtinho, D., Vitorino, C., Valente, A. J. M., Muniz, E. C., *DNA-containing PVA-based hydrogels for application in gene therapy*, 9th International Conference on Bio-based and Biodegradable Polymers - BIOPOL, Coimbra, 2024. **Poster**
12. Díaz-Puertas, R., Badía, P. V., Carrió, J. M., Murtinho, D., Valente, A. J. M., Mallavia, R., *Synthesis and characterization of a fluorescent derivative of PMVEMA with pyrene*, 9th International Conference on Bio-based and Biodegradable Polymers - BIOPOL, Coimbra, 2024. **Poster**
13. Ramos, A. R. A., Matias, P. M. C., Murtinho, D., Valente, A. J. M., *Synthesis and characterization of amine-rich cyclodextrin-based nanosponges for the removal of synthetic dyes*, 9th International Conference on Bio-based and Biodegradable Polymers - BIOPOL, Coimbra, 2024. **Poster**
14. Costa, T. B., Matias, P. M. C., Murtinho, D. M. B., Valente, A. J. M., Rosa, D. S., *Green composite hydrogels containing microcellulose from eucalyptus wastes to remove potentially toxic metals*, 9th International Conference on Bio-based and Biodegradable Polymers - BIOPOL, Coimbra, 2024. **Poster**

15. Sousa, J. F. M., Murtinho, D. M. B., Valente, Marques, J. M. C., *Remove of tetracycline by chitosan-based polymers*, 9th International Conference on Bio-based and Biodegradable Polymers - BIOPOL, Coimbra, 2024. **Poster**
16. Costa, T. B., Matias, P. M. C., Rosa, D. S., Murtinho, D. M. B., Valente, *Enhancing nanocelluloses modified with succinic anhydride for efficient removal of heavy metals in aqueous medium*, XXVIII Galician-Portuguese International Conference on Chemistry, Vigo, Spain, 2024. **Poster**
17. Fernandes, F. R. L., Soares, S. R., Azevedo, E. F. G., Ribeiro, A. C. F., *Coupled diffusion of analgesic drugs and caffeine in polymeric solutions*, XXVI Iberian Meeting on Colloids and Interfaces, RIC110, Coimbra, 2024). **Poster**
18. Jiménez, D. M. G., Vargas, E. F., Ribeiro, A. C. F., Estes, M.A., *Coeficientes de difusión y conductividades iónicas de soluciones acuosas de C-tetra(etil) resorcin[4]areno sulfonado y C-tetra(propil) resorcin[4]areno sulfonado*, XXVI Congresso Sociedade Ibero-americana de Electroquímica (SIBAE) Lisboa, 2024. **Poster**
19. Benavente, A. C., Galindres, D. M., Maldonado, M., Ribeiro, A. C. F., Estes, M. A., *Efecto del dodecilsulfato de sódio sobre la sulfadiazina sódica en disolución acuosa*, XXVI Congresso Sociedade Ibero-americana de Electroquímica (SIBAE) Lisboa, 2024. **Poster**
20. Pacheco, D., Silva-Barroso, A. S., Cancelli, G., Teles, H., Lourenço, M., Seabra, R., Valente, J., Montesi, M., Panseri, S., Sobral, A., Encarnação, T., Alves, N., Mateus, A., Gloria, A., Mota, C., Patrício, T. M. F., *3D-printed collagen-based scaffolds as suitable platform for bone tissue regeneration*, Conference on Collaborative Horizons: Shared Discoveries in Regenerative Medicine, Maastricht, The Netherlands, 16-18 October, 2024. **Poster**
21. Santos, F., Nicolau, N., Vargas, P., Gameiro, F., Lourenço, M., Pacheco, D., Patrício, T., Valente, J., Batista, C., Rodrigues, P. V., Machado, A., Massano, A., Mitchell, G. R., Mateus, A., Sobral, A. J. F. N., Encarnação, T., *Development and characterization of a novel fully bio-based material composite of PHBV, PLA, and chitosan*, 9th International Conference on Bio-Based & Biodegradable Polymers, Coimbra, Portugal, 22-24, July, 2024. **Poster**
22. Santos, F., Rodrigues, P., Vargas, P., Massano, A., Oliveira, L. M., Cruz, V., Mateus, A., Mitchell, G. R., Sobral, A. J. F. N., Encarnação, T., *A novel fully bio-based material composite for cosmetic packaging applications*, INOV.AM International Conference, Braga, Portugal, 27-28 November, 2024. **Poster**
23. Cotrim, C., Santos, B., Araújo, J., Sobral, A. J. F. N., Freitas, F., Bernardino, R., Encarnação, T., *Bioremediation of Endocrine-Disrupting Chemicals by marine microalgae Nannochloropsis sp.*, Encontro Ciência 2024, Porto, Portugal, 3 a 5 de julho de 2024. **Poster**
24. Santos, B., Araujo, J., Sobral, A., Freitas, F., Encarnação, T., *Development and validation of a RP-HPLC method for the simultaneous analysis of six Contaminants of Emerging Concern during microalgae bioremediation*, Third International Chemistry Conference, Lisbon, Portugal, June 17-19, (2024). **Poster**
25. Nunes Barradas, N., P. D., Murtinho, D., Seixas de Melo, J. S., *Chitosan polymer randomly labeled with pyrene: Synthesis, photophysics, and selective quenching by metal cations and anions*, X Iberian Meeting on Colloids and Interfaces (RICI X), Coimbra, Portugal, 2024. **Poster**
26. Nunes Barradas, P. D., Sérgio Seixas de Melo, J.S., Jötten, H. J., Nguyen, N. B., Scherf, U., *Photophysical and spectroscopic characterization of methyl-substituted ladder-type(meta-phenylene) compounds*, VIII Jornadas Ibéricas de Fotoquímica & I Franco-Iberian Conference on Photochemistry, Lisboa, Portugal, 2024. **Poster**
27. Cunha, C., Seixas de Melo, J. S., *Molecular Evolution: from Indigo to Isoindigo*, 29th PhotoIUPAC, IUPAC Symposium on Photochemistry, Valencia, Spain, 2024. **Poster**
28. Peixoto, M., Rodrigues, A. C., Pineiro, M., Seixas de Melo, J. S., *Aggregation-induced emission in asymmetric chalcone-substituted diphenylbenzofulvenes*, 29th PhotoIUPAC, IUPAC Symposium on Photochemistry, Valencia, Spain, 2024. **Poster**

29. Marques, J. M. C., *Structure, energetics, and thermodynamics of charged colloidal clusters modeled with isotropic potentials*, X Iberian Meeting on Colloids and Interfaces (RICI10), Coimbra, Portugal, 2024. **Poster**
30. Montagna, F. J. V., Camargo, G Camargo Solorzano, P., Soares, M. I. L., Pinho e Melo, T. M. V. D., Peláez, W. J., *Flash Vacuum Pyrolysis (FVP) of Dimethyl 5-Methyl-3-phenyl-1H,3H-pyrrolo[1,2-c]thiazole-6,7-dicarboxylate 2,2-Dioxide: Kinetic and Thermal Parameters*, II Southern Science Conference (SSCON), Mendoza, Argentina, 2024. **Poster**
31. Sousa, J. F. M., Murtinho, D., Valente, A. J. M., Marques, J. M. C., *Remove of tetracycline by chitosan-based polymers*, 9th International Conference on Bio-based and Biodegradable Polymers (BIOPOL2024), Coimbra, Portugal, 2024. **Poster**
32. Santos, C. I. A. V., Casaleiro, A. F., Jerónimo, S. B., Gramacho, S. A., Ramos, M. L., Gando-Ferreira, L. M., *Characterization of waste and regenerated lubricant oil – an efficiency study*, X Iberian Meeting on Colloids and Interfaces, 23-26 June, Coimbra, Portugal, 2024 **Poster**
33. Mendes, M., Cova, T., Nunes, S., Vitorino, C., Pais, A., *Integrating Machine Learning and Molecular Simulations to Enhance Cell-Penetrating Peptide-Modified Nanoparticles*, BIOPOL- 9th International Conference on Bio-based and Biodegradable Polymers Coimbra, Portugal, 22-24 July 2024. **Poster**
34. Ferreira, C. F., Cova, T. F., Nunes, S.C.C., Pais, A. A. C. C., *Exploring Molecular Descriptors for Mycotoxin Identification and Characterization through Machine Learning* , RICIX- 10th Iberian Meeting on Colloids and Interfaces, Coimbra, Portugal, 23 – 26 June, 2024. **Poster**
36. Nossa, A. R., Cova, T. F., Nunes, S.C.C., Pais, A. A. C. C., *Characterization of PFASs using machine learning and electronic structure calculations*, RICIX- 10th Iberian Meeting on Colloids and Interfaces, Coimbra, Portugal, 23 – 26 June, 2024. **Poster**
37. Nunes, S. C. C., Firmino, T., Pais, A. A. C. C., *DNA-based nanocages: shape and electrostatics*, RICIX- 10th Iberian Meeting on Colloids and Interfaces, Coimbra, Portugal, 23 – 26 June, 2024. **Poster**
38. Mendes, M., Sereno, J., Cova, T., Nunes, S., Fortuna, A., Castelo-Branco, M., Abrunhosa, A. J., Ramos, M. L., Sousa, J., Pais, A., Vitorino, C., *Surface matters: The delivery dilemma using lipid nanoparticles in glioblastoma*, RICIX- 10th Iberian Meeting on Colloids and Interfaces, Coimbra, Portugal, 23 – 26 June, 2024. **Poster**
39. Esteves, M.J.S., Cova, T. F. G. G., Nunes, S.C.C., Pais, A.A.C.C., *Antibiotics: identification and characterization using machine learning as a playground*, RICIX- 10th Iberian Meeting on Colloids and Interfaces, Coimbra, Portugal, 23 – 26 June, 2024. **Poster**
40. A.M.R. Pereira, A.H. Kakon, C. Serpa, L. Grosche, *“Sustainable Synthesis of High Purity Biosilica from Rice Husk: Overcoming the Limitations of Mineral Acid Leaching”*. XXVIII Encontro Galego-Portugués de Química, Vigo, Spain, 13-15 November 2024. **Poster**
41. A. Costa-Tuna, G. Ribeiro, A. Pereira, A.H. Kakon, O.A. Chaves, J.C. Netto-Ferreira, C. Serpa, *“Photodegradation of food dyes using bio-silica supported silver nanoparticles”*. 8th JIF Jornadas Ibéricas de Fotoquímica, 1st FICP Franco-Iberian Conference of Photochemistry, Lisbon, Portugal, 11-13, September 2024. **Poster**
42. D. Amado, O.A. Chaves, R. Loureiro, C.S. Jesus, P.F. Cruz, Z.L. Almeida, C. Serpa, R.M.M. Brito, *“Unravelling Protein Folding Dynamics with Photoacoustic Calorimetry: the case of Chignolin”*. 8th JIF Jornadas Ibéricas de Fotoquímica, 1st FICP Franco-Iberian Conference of Photochemistry, Lisbon, Portugal, 11-13, September 2024. **Poster**

43. A. Duque-Prata, L.G. Arnaut, C. Serpa, “*Pushing the Boundaries of Electron Transfer Reactions*”. 8th JIF Jornadas Ibéricas de Fotoquímica, 1st FICP Franco-Iberian Conference of Photochemistry, Lisbon, Portugal, 11-13, September 2024. **Poster**
44. O.A. Chaves, C. Serpa, “*The Nature of Charge on Porphyrin Structure Unexpectedly Stimulates the Aggregation of the Photosensitizer at the Surface of the Human Serum Albumin*”. 8th JIF Jornadas Ibéricas de Fotoquímica, 1st FICP Franco-Iberian Conference of Photochemistry, Lisbon, Portugal, 11-13, September 2024. **Poster**
45. A. Duque-Prata, C. Serpa, L.G. Arnaut, “*The Endless Surprises of Free-Energy Dependences of Electron Transfers*”. Gordon Research Conference Electron Donor-Acceptor Interactions, Newport (RI), USA, 28 July-3 August 2024. **Poster**
46. C. Serpa, A. Costa-Tuna, S. Gramacho, “*Photodegradation of ibuprofen using different gold nanoparticles shapes*”. 3rd Edition NanoSeries Conference on Global Nanotechnology (#NanoSeries2024,) Lisboa, Portugal, 17-19 June 2024. **Poster**
47. A. Costa-Tuna, G. Ribeiro, A. Pereira, A.H. Kakon, C. Serpa, “*Photodegradation of food dyes using silver nanoparticles supported in biosilica*”. 3rd Edition NanoSeries Conference on Global Nanotechnology (#NanoSeries2024,) Lisboa, Portugal, 17-19 June 2024. **Poster**
48. E. Seletchi, M. I. Mendes, D. A. Pereira, M. J. Moreno, M. J. F. Calvete, L. G. Arnaut, “*Phase-change contrast agents for photoacoustic tomography based on phthalocyanines*”. 22nd International Conference on Photoacoustic and Photothermal Phenomena, Coimbra, Portugal, 8-12 July 2024 **Poster**
49. Arnaut, Z. A., Cruz-Oliveira, C., Castanho, M. R. A. B., Pereira, M. M., *Study of structure-activity relationship of porphyrins on ZIKV inactivation*, ICPP, Buffalo, USA, 2024. **Poster**
50. Arnaut, Z. A., Felgueiras, A. P., Rodrigues, F., Aroso, R. T., Pais, A. A. C. C., Pereira, M. M., *Synthesis of various meso-aryl porphyrins using flow chemistry*, ICPP, Buffalo, USA, 2024. **Poster**
51. Gonzalez, A.C.S., Carrilho, R.M.B., Pereira, M.M., *Homogeneously Catalyzed Synthetic Approaches towards Functionalized Photosensitive CO₂-based Polycarbonates*, ISHC 2024 - XXIII International Symposium on Homogeneous Catalysis, Trieste, Italy, July 2024. **Poster**
52. Masliy, V., Takács, A. Carrilho, R.M.B., Pereira, M.M., Kollár, L., *One-pot halogen-selective dicarbonylation of 1-bromo-4-iodobenzene using pharmaceutically relevant nucleophiles*, ISHC 2024 - XXIII International Symposium on Homogeneous Catalysis, Trieste, Italy, 2024. **Poster**
53. Aroso, R. T.; Domingos, C. V.; Rodrigues, F. M. S.; Silva, G. J.; Carrilho, R. M. B.; Pereira, M. M., *Unraveling the Impact of Photosensitizer Structure on the Antibacterial Prowess of Photodecontaminant Biopolymers*, 13th International Conference on Porphyrins & Phthalocyanines (ICPP-13), Buffalo, United States of America, 2024. **Poster**
54. Anita S. Amorim, Zoe A. Arnaut, Mariette M. Pereira, Luís Arnaut, “*Use of a cationic di-imidazolyl chlorin for antimicrobial photodynamic therapy*”. PathBio, Galway, Ireland, 6-7 June 2024. **Poster**
55. Amílcar Duque-Prata; Carlos Serpa; Pedro J.S.B. Caridade, “*Resazurin derivatives for in vivo studies: spectroscopy, electrochemical and structural properties*”. Virtual Winter School for Computational Chemistry, Online, 29 January - 02 February 2024. **Poster**
56. Ntungwe, E., Roque, J. P. L., Nunes, C. M., Fausto, R., *Application of 1,2,4-Triazolium in Structural Modification of Natural Products and their Biological Activity Studies*, International Congress on Natural Products Research, Kraków, Poland, 2024. **Poster**
57. Sequeira, M. C. M., Nogueira, B. A., Nikitin, T., Caetano, F. J. P., Diogo, H. P., Fareleira, J. M. N. A., Fausto, R., *Thermophysical Properties of n-Alkane Systems for Low Temperature Thermal Energy Storage*, 22nd Symposium on Thermophysical Properties and 18th International Conference on the Properties of Water and Steam, Boulder, USA, 2024. **Poster**

58. [Braz, S.](#), Justino, L. L. G., Ramos, M. L., Fausto, R., *Indigo Carmine Food Dye (E132) Binding to Cu(II) in Aqueous Solution and Solid State: A Spectroscopic and DFT Characterization Study*, 10th Iberian Meeting on Colloids and Interfaces, Coimbra, Portugal, 2024. **Poster**
59. [Madeira, C.](#), Justino, L. L. G., Ramos, M. L., Costa, T., Fausto, R., *Alizarin Red S Complexes with Mo(VI) and Their Interaction with Cationic Surfactants: Potential for Applications in Sensing*, 10th Iberian Meeting on Colloids and Interfaces, Coimbra, Portugal, 2024. **Poster**
60. [Ildiz, G. O.](#), Nogueira, B. A., Fausto, R., *Overseeing Hydantoins: Structural, Vibrational and Photochemical Trends, and Substituent Effects*, XVII International Conference on Molecular Spectroscopy ICMS 2024, Wojanów, Poland, 2024. **Poster**
61. [Castro, R. A. E.](#), Puppini, L., Baptista, J. A., Canotilho, J., Eusébio, M. E. S., *New solid forms of sotagliflozin, From Molecules to Materials: 1st workshop on benchmarking solid state properties, Bringing Experiment and Simulation Together in Crystal Structure Prediction - COST ACTION CA22107*, Warsaw, Poland, 2024. **Poster**
62. [Baptista, J. A.](#), Castro, R. A. E., Fantechi, E., Chelazzi, L., Ciattini, S., Rosado, M. T. S., Eusébio, M. E. S., *Polymorphism of Probuconol and Structurally Related Compounds, From Molecules to Materials: 1st workshop on benchmarking solid state properties, Bringing Experiment and Simulation Together in Crystal Structure Prediction - COST ACTION CA22107*, Warsaw, Poland, 2024. **Poster**
63. [Silva, J. F. C.](#), Pereira, P. S., Silva, M. R., Eusébio M. E. S., Rosado, M. T. S. *Domperidone co-amorphous phases with xanthine derivatives*, Multiscale Phenomena in Condensed Matter, MULTIS 2024, Krakow, Poland, 2024. **Poster**
64. [Serrão, G.](#), Scarpelli, F., Rosado, M., Crispini, A., *Quinolines as optimal Halogen-Bonding acceptors*, 34th European Crystallographic Meeting ECM34, Padova, Italy, 2024. **Poster**
65. [Chelazzi, L.](#), Ciattini, S., Fantechi, E., Silva, J. F. C., Silva, P. S. P., Silva, M. R., Eusebio, M. E. S., Rosado, M. T. S., *Ranolazine: crystal structure determination and investigation of its metastable polymorphs*, 34th European Crystallographic Meeting ECM34, Padova, Italy, 2024. **Poster**
66. Cardoso, A. L., Sousa, J. C., Fonseca, L., Pinho e Melo, T. M. V. D., Pineiro, M., *Mechanochemical transformations of furans: sustainability meets diversity*, 29th Congress of the International Society of Heterocyclic Chemistry (ISHC 2024), Aveiro, Portugal, 21-26 de julho de 2024. **Poster**
67. Soares, M. I. L., Pinho e Melo, T. M. V. D., *Phosphine-catalyzed umpolung γ -addition of iminochromanes to allenes: synthesis of functionalized 2H-chromenes*, 29th Congress of the International Society of Heterocyclic Chemistry (ISHC 2024), Aveiro, Portugal, 21-26 de julho de 2024. **Poster**
68. Simões, J. C. S., Domingues, T. M., Rodrigues, A. C. B., Seixas de Melo, J. S., Pineiro, M., Pinho e Melo, T. M. V. D., *Novel trans-A2B2 porphyrins: from oxime meso-substituted dipyrromethanes to functionalized macrocycles*, 29th Congress of the International Society of Heterocyclic Chemistry (ISHC 2024), Aveiro, Portugal, 21-26 de julho de 2024. **Poster**
69. Costa, B. D. P., Mestre, C., Rodrigues, A. C. B., Pineiro, M., Seixas de Melo, J. S., Botelho, M. F., Lopes, S. M. M., Laranjo, M., Pinho e Melo, T. M. V. D., *Photodynamic therapy of endometrial cancer: improving the properties of corrole photosensitizers by exploring fluorine effects*, 29th Congress of the International Society of Heterocyclic Chemistry (ISHC 2024), Aveiro, Portugal, 21-26 de julho de 2024. **Poster**
70. Carvalho, R. M., Gonçalves, J. V. R., Gonçalves, P., Alves, A. J. S., Bártolo, I., Taveira, N., Pinho e Melo, T. M. V. D., *Novel spiropenicillanates via formal [2+1] cycloaddition of 6-alkylidenepenicillanates with sulfur ylides*, 29th Congress of the International Society of Heterocyclic Chemistry (ISHC 2024), Aveiro, Portugal, 21-26 de julho de 2024. **Poster**

71. Alves, A. J. S., Castro, B. J. L., Alves, N. G., Bártolo, I., Taveira, N., Pinho e Melo, T. M. V. D., *Novel sulfoxide- and sulfone-spiroenicillanates with potential broad-spectrum antiviral activity*, 29th Congress of the International Society of Heterocyclic Chemistry (ISHC 2024), Aveiro, Portugal, 21-26 de julho de 2024. **Poster**
72. Amorim, A. C., Morgado, J., Burke, A. J., Gomes, H. *Electrical Characterization of Novel Phthaloperinones for Organic Electronics*, 245th ECS Meeting, San Francisco, USA, 26-30 de maio, 2024. **Poster**
73. Barradas, P. D. N., Murtinho, D., Seixas de Melo, J. S., *Chitosan polymers randomly labeled with pyrene: synthesis, photophysics, and selective quenching by metal cations and anions*, X Iberian Meeting on Colloids and Interfaces (RICI X), 23–26 June, Coimbra, Portugal, 2024. **Poster**
74. Esteves, M. I. M., Murtinho, D., Henriques, C. A., Antunes, F. E., *Amino Acid-based Surfactants Derived from Used Cooking Oils: The Pursue for a Sustainable Synthesis*, X Iberian Meeting on Colloids and Interfaces (RICI X), 23–26 June, Coimbra, Portugal, 2024. **Poster**
75. Sousa, J. F. M., Murtinho, D., Valente, A. J. M., Marques, J. M. C., *Removal of tetracycline by chitosan-based polymers*, 9th International Conference on Bio-based and Biodegradable Polymers (BIOPOL 2024), 22–24 July, Coimbra, Portugal, 2024. **Poster**
76. Camargo Solorzano, P., Soares, M. I. L., Pinho e Melo, T. M. V. D., Peláez, W. J., *Theoretical Study of SO₂ Extrusion Reaction for the Production of Diazafulvenium Methides and its Cycloaddition Reaction with Several Dipolarophiles*, II Southern Science Conference (SSCON), Mendoza, Argentina, 2024. **Poster**
77. Pinilla Peña, D. C., Soares, M. I., Pierella, L. B., Pinho e Melo, T. M. V. D., Peláez, W. J., *Thermal Reactions of 2,2-Dioxo-1H,3H-Pyrrolo[1,2-c]thiazoles Studied from Green Metrics*, II Southern Science Conference (SSCON), Mendoza, Argentina, 2024. **Poster**
78. Cordeiro, M. M., Filipe, H. A. L., Ramalho, J. P. P., Loura, L. M. S., Santos, P., Samelo, J., Moreno, M. J., *Hoechst 33342 acid/base properties and interaction with POPC membranes*, European South Atlantic Biophysics Congress ESAB2024, 4-7/06/2024, San Sebastian, Espanha. **Poster**
79. Cordeiro, M. M., Salvador A., Moreno M. J., *Exploring Labetalol Permeation Across Lipidic Membranes: Insights from the pH Variation Assay*, European South Atlantic Biophysics Congress ESAB2024, 4-7/06/2024, San Sebastian, Espanha. **Poster**
80. Galdes, C. F. G. C., Pinto, S. M. A., Teixeira, D. S. S., Garda, Z., Pallier, A., Tóth, É., Pereira, M. M., *Optimization of Fluorinated Mn(III)/(II)-Porphyrins as Redox-Responsive ¹⁹F and ¹H NMR Relaxation Probes*, 19th European Molecular Imaging (ESMI) Meeting (EMIM 24), 12-15/03/2024, Porto, Portugal. **Poster**
81. Griffith, M., Araújo, A., Travasso, R., Salvador, A. *Spatially localized redox relays allow sensitive and site-specific hydrogen peroxide signaling in human cells*. Thiol-Based Redox Regulation and Signaling Gordon Research Conference, 14-19/07/2024, Castelldefels, Espanha. **Poster**
82. Griffith, M., Araújo, A., Travasso, R., Salvador, A. *Redox-induced spatial and functional differentiation of the peroxiredoxin/thioredoxin system in the cytosol of human cells*. European South Atlantic Biophysics Congress ESAB2024, 4-7/06/2024, San Sebastian, Espanha. **Poster**
83. Mahmoud, A. G., Librando, I., Paul, A., Carabineiro, S. A. C., Ferraria, A. M., Botelho do Rego, A. M., Guedes da Silva, M. F. C., Galdes, C. F. G. C., Pombeiro, A. J. L., *Novel organotin-PTA complexes supported on carbon materials as recyclable catalysts for solvent-free cyanosilylation of aldehydes*, EurASc Symposium & Ceremony, Academia de Ciências de Lisboa, Lisboa, 29-30/10/2024, Portugal, **Poster**
84. Ramos, C. V., Raynold A. A., Ferreira, L., Moreno M. J., *From Synthesis to Characterization: Exploring the Impact of Polymer Brush Coating on Liposomal Membranes*, 10th Iberian Meeting on Colloids and Interfaces RICI X, 23-26/06/2024, Coimbra, Portugal. **Poster**

CQC – Overall Output Indicators 2024

85. Sánchez-Martín, V., Machado, F., Coimbra, M. A., Coreta-Gomes, F., del Castillo, M. D., *Effect of in vitro human colonic fermented coffee melanoidins on colon cancer cell proliferation*, 5th International Electronic Conference on Foods, 28-30/10/2024. **Poster**

86. Silva, M. I., Foulquié, E., Fonseca, A., Rodrigues, M. C., Sebastião, F., Vieira, J., Vaz, D.C., Pereira, C., Guimarães, C., Ribeiro, V.S., *Antioxidant and antimicrobial properties of extracts of wild and commercialized Mentha pulegium L.*, International Conference on Water Energy Food and Sustainability (ICoWEFS 2024), 8-10/5/2024, Portalegre, Portugal, 2024. **Poster**

87. Streit, J. O., Cassaignau, A. M., Chan, S. H. S., Bukvin, I. V., Wlodarski, T., Waudby, C. A., Cabrita, L. D., Figueiredo, A. M., Christodoulou, J., *The effect of the ribosome on the conformational ensemble of an unfolded nascent chain*, European Magnetic Resonance Congress EUROMAR, 30/6-4/7/2024, Bilbao, Espanha. **Poster**

88. Teixeira, D. S. S., Garda, Z., Pallier, A., Geraldes, C. F. G. C., Pinto, S. M. A., Pereira, M. M., Jakab-Tóth, É., *Water-Soluble, Fluorinated Manganese Porphyrin Complexes for Redox Detection*, The Future of Molecular MR, 17-20/06/2024, Orléans, França. **Poster**

Communications at National Meetings (86)

National Keynotes / Plenary / Invited Lectures (21)

1. Valente, A. J. M., “Cyclodextrin nanosponges”. 3º Encontro RT4/CIQUP/IMS, Porto, 2024 **Invited Keynote**.
2. Seixas de Melo, J. S., *Bright and Dark Molecules: A Photophysical Journey*, 16th National Physical Chemistry Meeting (ENQF), Faculdade de Ciências da Universidade de Lisboa, Lisboa, 7-19 July 2024. **Invited Lecture**
3. Luis G. Arnaut. “O Som da Luz: do Fotofone à Transfeção de Genes”. X Encontro Nacional de Estudantes de Química, 22-24/03/2024, Covilhã. **Lição plenária**
4. Lúcia C. Gomes-da-Silva “MedLife Thematic Line” – Open Day IMS - Institute of Molecular Sciences, Coimbra, Portugal, 10 October 2024 **Invited Lecture**
5. Carrilho, R.M.B., *Sustainable Catalytic Processes for CO₂ Valorization*, XII ENCMP - XII National Meeting on Catalysis and Porous Materials, Coimbra, Portugal, 2024. **Invited Lecture**
6. Pereira, M.M., *Sustainable and Scalable Processes for Fine Chemicals*, IST, Lisboa, 2024. **Plenary Lecture**.
7. Rodrigues F. M. S., *Development of catalytic continuous flow processes: synthesis of fine chemicals*, Summer School – Process intensification by flow chemistry, Faculty of Pharmacy, University of Lisbon, Lisboa, Portugal, 2024. **Invited Oral Presentation**
8. Pereira, M. M., *Perspectives on catalytic continuous flow process in fine chemical industry*, 15th National Organic Chemistry Meeting & 8th National Medicinal Chemistry Meeting, Faro, 2024. **Invited Oral Presentation**
9. Pinto, S.M.A., Teixeira, D.S.S., Geraldes, C.F.G.C., Tóth, E., Pereira, M.M., 14th Inorganic & Bioinorganic Chemistry Conference, Lisboa, Portugal, 2024. **Invited Lecture**.
10. Castro, R. A. E., *Estado sólido de ativos farmacêuticos*, Núcleo de Estudantes de Química da Universidade do Porto, Porto, Portugal, 2024. **Invited Lecture**
11. Silva, J. F. C., Eusébio, M. E. S., Rosado, M. T. S., *How to avoid crystallization pits on the energy landscapes of amorphous drugs*, 30 minutos de Química, Department of Chemistry, University of Coimbra, 2024. **Invited Oral Presentation**
12. Viegas, L. P., *Computational Chemistry at the service of Green Chemistry*". Palestra convidada online nas sessões bluejournalclub da Bluepharma, Coimbra, Portugal, 17 Abril 2024. **Plenary Lecture**
13. Rodrigues, S.P.J., *Evocações químicas na literatura: da banalidade ao maravilhoso*, 15.ª edição de Contornos da Palavra/Encontro de Bibliotecas Escolares, Viana do Castelo, Portugal, 2024. **Invited Lecture**
14. Pineiro, M., *Mechanochemistry: in search of sustainable methods for the synthesis of heterocycles* 15º Encontro Nacional de Química Orgânica e 8.º Encontro Nacional de Química Medicinal, Faro, Portugal, 2024. **Keynote Lecture**
15. Geraldes, C.F.G.C., *Paramagnetic complexes as sensors for biomedical MRS and MRI*, 4th Inorganic & Bioinorganic Chemistry Conference (2024 IBiCC), 16-18/05/2024, Lisboa, Portugal, **Invited Oral Presentation**

CQC – Overall Output Indicators 2024

16. Moreno, M. J., *Bioactive Molecules and Biomembranes: A Pathway to Predicting Drug Behavior in vivo*, Webinar integrado no ciclo de conferências intitulado “Químicas” e organizado pela Sociedade Portuguesa de Química, https://www.spq.pt/quimicas_ciclo_conferencias, 30/10/2024, **Invited Oral Presentation**
17. Moreno, M. J., *Challenges and Opportunities in ITC: Thermodynamics of Molecular Interactions and Beyond, Exploring Biomolecular Landscapes: Insights from Biophysical Characterization Techniques* (organized by Paralab bio), Instituto de Medicina Molecular, 2/10/2024, Lisboa, Portugal, **Invited Oral Presentation**
18. Pinto, S. M. A., Teixeira, D. S. S., Geraldes, C.F.G.C., Tóth, E., Pereira, M. M., *Manganese(III/II)-water soluble fluorinated tetrapyrrolic macrocycles as potential redox MRI probes*, 4th Inorganic & Bioinorganic Chemistry Conference (2024 IBiCC), 16-18/05/2024, Lisboa, Portugal, **Invited Oral Presentation**
19. Ramos, M. J., Geraldes, C. F. G. C. , *O Prémio Nobel de Química 2024*, Academia de Ciências de Lisboa, 20/10/2024, Lisboa, Portugal, **Invited Oral Presentation**
20. Salvador, A., *Reaction-diffusion modeling of H₂O₂ signaling in human cells*, Reunião da comunidade de *microbial biotechnology and systems biology* do Biodata.pt, 24/11/2024, online, **Invited Oral Presentation**
21. Pineiro, M., *Mechanochemistry and catalysis, a powerful alliance for the development of sustainable processes*, XII Encontro Nacional de Catálise e Materiais Porosos, Coimbra, Portugal, 2024. **Invited Oral Presentation**

National Oral Presentations (19)

1. Matias, P. M. C., Rodrigues, Murtinho, D., Valente, A. J. M., *Triazine porous organic polymers for simultaneous removal and sensing of antibiotics in water*, 16th National Physical Chemistry Meeting, Lisboa, Portugal, 2024. **Oral Presentation - Awards for best Oral Communication**
2. Sousa, J. F. M., Murtinho, D., Valente, A. J. M., Marques, J. M. C., *Chitosan and naphthaldehydes derivatives composites: adsorptive remove of tetracycline from water*, 16th National Physical Chemistry Meeting, Lisboa, Portugal, 2024. **Oral Presentation**
3. Machado, F., Laronha, H., Coelho, E., Nunes, C., Coimbra, M., Coreta-Gomes, F., *Cholesterol lowering foods: a quest towards a functional ingredient*, XVII Encontro de Química Alimentar, 9-11/10/2024, UTAD, Portugal. **Comunicação oral.**
4. Santos, J. R. C., Abreu, P. E., Marques, J. M. C., *Unveiling pesticide interactions: Insights from the *Aplysia californica* AchBP-imidacloprid complex*, 16th National Physical Chemistry Meeting, Lisboa, Portugal, 2024. **Oral Presentation**
5. Gil, J., Sobral, A., *Armazenamento de Hidrogénio em TiO₂ mesoporoso*, Zoom para a UC Business Universidade de Coimbra, 13 de março de 2024. **Oral Presentation**
6. Jesus, C., Murtinho, D., Alves, A., Antunes, F., *Physico-chemical Characterization of N-alkyldimethylglucosylammonium iodide: new sugar-based cationic surfactants*, RICI X, Coimbra, Portugal, junho 2024. **Oral Presentation**
7. Sousa, F., Grosche L., Antunes, F., *Rice Husk as reinforcement fibre for PLA and PBS-based composites*, RICI X, Coimbra, Portugal, 2024. **Oral Presentation**
8. Esteves, C., Antunes, F., Lindman, B., *Polycaprolactone-bassed shell materials for microcapsule applications*, BIOPOL, Coimbra, Portugal, 2024. **Oral Presentation.**
9. A. Amílcar Duque-Prata; Carlos Serpa; Pedro J.S.B. Caridade, “*Como usar a DFT para Determinar Potenciais Redox de Compostos Orgânicos*”
X Encontro Nacional de Estudantes de Química, Covilhã, Portugal, 23-24 March 2024. **Oral Presentation**
10. Gonzalez, A.C.S., Carrilho, R.M.B., Pereira, M.M., *Highly selective phthalocyanine-based catalysts for CO₂ addition reactions to epoxides*, XII ENCMP - XII National Meeting on Catalysis and Porous Materials, Coimbra, Portugal, 2024. **Oral Presentation**
11. Rodrigues F. M. S., Carrilho, R. M. B., Calvete, M. J. F., Kollár, L., Pereira, M. M., *Pd-catalyzed aminocarbonylation continuous-flow process: Multigram synthesis of carboxamides*, XII Encontro da Divisão de Catálise e Materiais Porosos da Sociedade Portuguesa de Química, Coimbra, Portugal, 2024. **Oral Presentation**
12. Domingos, C. V., Rodrigues, F. M. S., Tavares, I., Aroso, R. T., Calvete, M. J. F., Pereira, M. M. *Shining Against Resistance: Photodecontaminant Materials for inactivation of Bacteria*, 15th National Organic Chemistry Meeting and 8th National Medicinal Chemistry Meeting, Faro, Portugal, January 2024. **Oral presentation.**
13. Duarte, L. J., Nunes, C. M., Fausto, R., Braga, A. A. C., *Investigation of the IVR Isomerization of Nitrous Acid*, 16th National Physical Chemistry Meeting, Lisboa, Portugal 2024. **Oral Presentation**
14. Bouznif, H., Justino, L. L. G., Soares, M. I. L., Costa, T., Ramos, M. L., Nikitin, T., Pinho e Melo, T. M. V. D., Zouari, N., Fausto, R., *A Combined Structural, Spectroscopic, and Theoretical Investigation of a Water-Soluble Schiff Base: Stability and Enol-Imine/Keto-Enamine Tautomerism*, 16th Encontro Nacional de Química-Física da SPQ, Lisboa, Portugal, 2024. **Oral Presentation**

CQC – Overall Output Indicators 2024

15. Viegas, L. P., *Constrained Transition State Randomization: A general transition state sampling method for bimolecular reactions*. XVI Encontro Nacional de Química Física/V Simpósio de Química Computacional, Lisboa, Portugal, 17-19 Julho 2024. **Oral Presentation**

16. Soares, M. I. L., Pinho e Melo, T. M. V. D., *Lewis Base-Catalyzed Reactions of Chromans and Allenolates: Access to Structurally Diverse Chroman Frameworks*, 15° Encontro Nacional de Química Orgânica (15ENQO) / 8° Encontro Nacional de Química Medicinal & Química Biológica (8ENQT), Faro, Portugal, 2024. **Oral Presentation**

17. Braz, J., Lopes, S. M. M., Laranjo, M., Pineiro, M., Botelho, M. F., Pinho e Melo, T. M. V. D., *Oxime-functionalized trans-A2B-corroles as promising photosensitizers for photodynamic therapy of lung cancer*, 15° Encontro Nacional de Química Orgânica (15ENQO) / 8° Encontro Nacional de Química Medicinal & Química Biológica (8ENQT), Faro, Portugal, 2024. **Flash Presentation**

18. Bouznif, H., Justino, L. L. G., Soares, M. I. L., Costa, T., Ramos, M. L., Nikitin, T., Pinho e Melo, T. M. V. D., Zouari, N., Fausto, R., *A Combined Structural, Spectroscopic, and Theoretical Investigation of a Water-soluble Schiff Base: Stability and Enol-imine/keto-enamine Tautomerism*, 16th National Physical Chemistry Meeting (16ENQF) and 5th Computational Chemistry Symposium", Faculdade de Ciências, Universidade de Lisboa, Portugal, 2024. **Oral Presentation**

19. Costa F., Roque, A., Vaz, D.C., Pereira, S.G., *Bactérias comensais de doentes celíacos apresentam diferentes perfis de proteólise de gliadina in vitro*, 10 anos do Centro de Investigação da Unidade Local de Saúde da Região de Leiria, Escola Superior de Saúde de Leiria, 13-14/05/2024, Leiria, Portugal **Oral Presentation**

National Posters (46)

1. J. Varela, P. M. G. Nicolau, A. Messias, A. C. F. Ribeiro, A. J. M. Valente, S. I. G. Fangaia, *Libertação de iões de cobalto de ligas metálicas biomédicas de Co-Cr, estudo in vitro*, XLIV Congresso Anual da Sociedade Portuguesa de Estomatologia e Medicina Dentária (SPEMD) Porto, 11 a 12 de outubro de 2024 **Poster**
2. Gil, J., Dias, C., Sobral, A., *HYDROGEN STORAGE*, Apresentação na avaliação do Centro de Física da Universidade de Coimbra, novembro de 2004. **Poster**
3. Costa, T. B., Matias, P. M. C., Rosa, D. S., Murtinho, D. M. B., Valente, A. J. M., *Enhancing potato starch beads for effective sorption of toxic metals: the role of crosslinking degree*, 16th National Physical Chemistry Meeting, Lisboa, Portugal, 2024. **Poster**
4. Varela, J., Nicolau, P. M. G., Ribeiro, A. C. F., Valente, A. J. M., Fangaia, S. I. G., *Libertação de iões de cobalto de ligas metálicas biomédicas de Co-Cr – estudo in vitro*, Reunião Anual de Medicina Dentária e Estomatologia de Coimbra. Coimbra, 2024. **Poster**
5. Costa, T., Pineiro, M., Laranjo, M., Serambeque, B., Botelho, M. F., Pereira, N. A. M., Alves, A. J. S., Pinho e Melo T. M. V. D., Seixas de Melo, J. S., *Fluorescence/Phosphorescence Imaging Lifetime Microscopy Study on a Ratiometric Pt(II) Chlorine Oxygen Sensor*, 16º Encontro Nacional de Química Física + V Simpósio de Química Computacional, 17-19 Julho, Lisboa, Portugal, 2024. **Poster**
6. Marques, J. M. C., Zergani, F., Bartolomei, M., Pirani, F., *Energetics and structures of borophene nanoclusters*, X Iberian Meeting on Colloids and Interfaces (RICI10), Coimbra, Portugal, 2024. **Poster**
7. Santos, C. I. A. V., Casaleiro, A. F., Jerónimo S. B., Ramos, M. L., Gando Ferreira, L. M., *Evaluation of a green regeneration technology for waste lubricating oil*. Encontro Ciência 2024, 3-5 julho, Porto, Portugal, 2024. **Poster**
8. Dulyanska, Yuliya, Speck, A. D. D. P., Batista de Carvalho, L. A. E., Barroca, João, M. Gonçalves, F. J., Guiné, R. P. F., Santos, C. I. A. V., *Supercritical fluid extraction of bioactive compounds from Crataegus monogyna*, X Encontro Científico do NEQ/AAC, Coimbra, Portugal 2024. **Poster**
9. Esteves, M., Murtinho, D., Henriques, C., Antunes, F., *Aminoacid based surfactants derived from used cooking oils: the pursue for a sustainable synthesis*, RICI X, Coimbra, Portugal, 2024. **Poster**
10. Jesus, J., Esteves, C., Antunes, F., Santos, S., *Exploring the potential of bacterial cellulose films from SCOBY in Green Tea Kombucha*, Biopol, 22-24 julho 2024. **Poster**
11. R.S. Cunha, O.A. Chaves, P. Cruz, Z.L. Almeida, T. Costa, C. Serpa, *“Have you had your coffee today? The Impact of Caffeine on the Interactive Profile between Selected Commercial Drugs and Plasmatic Albumin”*. Biophysics Festival, Covilhã, Portugal, 9-10 May 2024.
12. O.A. Chaves, M.A.G. Soares, P.A. Aquino, T. Costa, C. Serpa, *“Insights into the Effect of Glucose on the Binding between Human Serum Albumin and the Nonsteroidal Anti-inflammatory Drug Nimesulide”*. Biophysics Festival, Covilhã, Portugal, 9-10 May 2024.
13. A.M.R. Pereira, A.H. Kakon, C. Serpa, L. Grosche, *“Synthesis of High Purity Biosilica from Rice Husk: Evaluating the Efficiency of Key Pretreatment Methods”*. Open Day IMS - Institute of Molecular Sciences, Coimbra, Portugal, 10 October 2024.
14. Felgueiras, A.P., Rodrigues, F.M.S., Masliy, V., Silva, M.F.C, Carrilho, R.M.B., Pereira, M.M., *Continuous flow sequential catalytic processes for scalable production of eugenol derivatives*, XII ENCMP - XII National Meeting on Catalysis and Porous Materials, Coimbra, Portugal, 2024.

CQC – Overall Output Indicators 2024

15. Masliy, V., Matos, R., Carrilho, R.M.B., Pereira, M.M., Fernandes, D.M., Peixoto, A.F., *Shrimp shells derived Pd/N-doped biochar for (electro)catalytic applications*, XII ENCMP - XII National Meeting on Catalysis and Porous Materials, Coimbra, Portugal, 2024.

16. Zomorodbakhsh, S., Cruz, I.G., Ferreira, F.S., Peixoto, A.F., Gil, J.M., Calvete, M.J.F., Pereira, M.M., Carrilho, R.M.B., *Functionalized biochars as efficient CO₂ adsorbents and renewable catalysts in cycloaddition to epoxides*, XII ENCMP - XII National Meeting on Catalysis and Porous Materials, Coimbra, Portugal, 2024.

17. Brás, E. M., Fausto, R., Cristiano, M. L. S., *Radicals at Very Low Temperatures: Monitoring Reactions and Interactions through IR Spectroscopy*, 15th National Organic Chemistry Meeting & 8th National Medicinal Chemistry Meeting, Faro, Portugal, 2024. **Poster**

18. Brito, A. L. B., Montargil, C., Duarte, C., Fausto, R., *Analysis of Plant-based Beverages Using Attenuated Total Reflectance Fourier-Transform Infrared Spectroscopy (ATR) Associated with Principal Component Analysis (PCA)*, Analítica 2024 – 11th meeting of the Analytical Chemistry Division of the Portuguese Chemical Society, Porto, Portugal, 2024. **Poster**

19. Ildiz, G. O., Nogueira, B. A., Fausto, R., *Structural, Vibrational and Photochemical Data of Simple Hydantoins – Common Features and Substituents Effects*, 16th Encontro Nacional de Química-Física da SPQ, Lisboa, Portugal, 2024. **Poster**

20. Nikitin, T., Lopes, S., Fausto, R., *Exploring Material Dynamics with Raman Spectroscopy at LRSM: Phase Transitions, Nanocomposites, Molecular Crystals, Peptides, Spherulites, and Graphene Oxide Reduction*, IMS Open Day, Coimbra, Portugal, 2024. **Poster**

21. Castro, R. A. E., Puppini, L., Baptista, J. A., Canotilho, J., Eusébio, M. E. S., *Investigation of solid forms of sotagliflozin*, 16^o Encontro Nacional de Química Física + V Simpósio de Química Computacional, Lisbon, 2024. **Poster**

22. Baptista, J.A., Castro, R.A.E., Canotilho, J., Rosado, M.T.S., Eusébio, M.E.S., *Thermodynamic and kinetic parameters of the crystallization of probucol and structurally related compounds from ethanol solutions*, 16^o Encontro Nacional de Química Física + V Simpósio de Química Computacional, 17-19 julho, Lisboa, (2024). **Poster**

23. Silva, M. I. G., Baptista, J. A., Castro, R. A. E., Eusébio, M. E. S., Canotilho, J., Maria, T. M. R., *Enhancing the Baricitinib Intrinsic Dissolution Rate by Co-crystallization and Amorphization*, 16^o Encontro Nacional de Química Física + V Simpósio de Química Computacional, Lisbon, 2024. **Poster**

24. Inácio, P. M. S., Baptista, J. A., Maria, T. M. R., Castro, R. A. E., Eusébio, M. E. S., Canotilho, J., *Modification of carprofen palatability via formation of multicomponent solid forms*, 16^o Encontro Nacional de Química Física + V Simpósio de Química Computacional, Lisbon, 2024. **Poster**

25. Porto, M. V., Castro, R. A., Rosado, M. T. S., Caires, F. J., *Cryomilling: A eficácia de baixas temperaturas de síntese na obtenção de sistema coamorfo*, Congresso Brasileiro de Engenharia e Ciência dos Materiais, Fortaleza, Brasil, 2024. **Poster**

26. Silva, J. F. C., Silva, P. S. P., Silva, M. R., Eusébio, M. E. S., Rosado, M. T. S., *Molecular synthon competition in domperidone amorphous systems*, Institute of Molecular Sciences (IMS) Open Day, 18 October, 2024. **Poster**

27. Américo J. S. Alves, João A. D. Silvestre, Teresa M. V. D. Pinho e Melo, *Continuous Flow Phosphine-Catalyzed [3+2] Annulation of Allenolates: Towards Efficient Synthesis of Chiral Spirocyclopentene-Penicillanates*, 15^o Encontro Nacional de Química Orgânica (15ENQO) / 8^o Encontro Nacional de Química Medicinal & Química Biológica (8ENQT), 20-24 janeiro, Faro, Portugal, 2024. **Poster**

28. Terver J. Sase, Ana L. Cardoso, Teresa M. V. D. Pinho e Melo, *Novel chiral organocatalysts for the asymmetric synthesis of 2-(tetrazol-5-yl)-2H-azirines*, 15^o Encontro Nacional de Química Orgânica (15ENQO) / 8^o Encontro Nacional de Química Medicinal & Química Biológica (8ENQT), 20-24 janeiro, Faro, Portugal, 2024. **Poster**

29. Joséia C. Sousa, Luana Fonseca, Teresa M. V. D. Pinho e Melo, Ana L. Cardoso, Marta Pineiro, *Mechanochemistry: A way to improve sustainability of furans' transformations*, 15^o Encontro Nacional de Química Orgânica (15ENQO) / 8^o Encontro Nacional de Química Medicinal & Química Biológica (8ENQT), 20-24 janeiro, Faro, Portugal, 2024. **Poster**
30. João C. S. Simões, Susana M. M. Lopes, Ana C. Beltran Rorigues, J. Sérgio Seixas de Melo, Marta Pineiro, Teresa M. V. D. Pinho e Melo, *Novel trans-A2B2 Porphyrins: From Oxime/Hydrazone α -Substituted Dipyrromethanes to meso-Substituted Functionalized Macrocycles*, 15^o Encontro Nacional de Química Orgânica (15ENQO) / 8^o Encontro Nacional de Química Medicinal & Química Biológica (8ENQT), 20-24 janeiro, Faro, Portugal, 2024. **Poster**
31. Susana M. M. Lopes, Teresa M. V. D. Pinho e Melo, *Hetero-Diels-Alder Reactions of a Novel Steroidal Nitrosoalkene*, 15^o Encontro Nacional de Química Orgânica (15ENQO) / 8^o Encontro Nacional de Química Medicinal & Química Biológica (8ENQT), 20-24 janeiro, Faro, Portugal, 2024. **Poster**
32. Carla Carvalho, Joana B. Loureiro, Tiago Ferreira, Adelina Quaresma, Paula A. Oliveira, Alberto Inga, Teresa M. V. D. Pinho e Melo, Lucília Saraiva, *Quimioprevenção de danos na pele induzidos por radiação ultravioleta através da reativação de mutantes da p53*, 6^o Encontro Nacional Jovens Investigadores em Oncologia (6^o ENJIO), 24 setembro, Porto, Portugal, 2024. **Poster**
33. Almeida, Z.L. & Rui M. M. Brito, *Removal of aberrant aggregates in amyloid diseases: from in silico analysis to in vitro biological activity*, IMS Open Day, 18th October, Coimbra, Portugal, 2024. **Poster**
34. Arranca, M. I., Coreta-Gomes, F., Coimbra, M. A., Coelho, E., Development of functional ingredients based on mushroom β -Glucans, XVII Encontro de Química Alimentar, 9-11/10/2024, UTAD, Portugal (best poster award). **Poster**
35. Cordeiro, M.M., Filipe, H. A. L. F., Ramalho, J. P. P., Loura, L. M. S., Santos, P., Samelo, J., Moreno, M. J., *Properties and Interaction of Hoechst 33342 with POPC Membranes*, Biophysics Festival, 4th Meeting of Young Biophysicists 4BF, 9-10/05/2024, Covilhã, Portugal. **Poster**
36. Ferreira, M. J., Rodrigues, T. A., Pedrosa, A. G., Gales, L., Salvador, A., Francisco, T., Azevedo, J. E., *Glutathione to the rescue: the importance of glutathione in mammalian peroxisomal redox homeostasis*, XXII National Congress Of Biochemistry, 24-26/10/2024, Aveiro, Portugal. **Poster**
37. Itacarambi, A., Salvador, A., Travasso, R. D. M., *Modeling H₂O₂ release and transport in the extracellular medium of tissues*, Biophysics Festival, 4th Meeting of Young Biophysicists 4BF, 9-10/05/2024, Covilhã, Portugal. **Poster**
38. Laronha, H., Coreta-Gomes, F., Coimbra, M. A., Coelho, C. *Hypocholesterolemic Potential of Mushroom Polysaccharides: Key Structure- Function Relationships*, 4th International Conference on Natural Products and Human Health, Aveiro University, 18-20/9/2024. **Poster**
39. Laronha, H., Coreta-Gomes, F., Coimbra, M. A., Coelho, E. *Assessment of cholesterol-lowering effects of mushrooms*, XXII National Congress Of Biochemistry, 24-26/10/2024, Aveiro, Portugal (best poster award). **Poster**
40. Laronha, H., Coreta-Gomes, F., Coimbra, M. A., Coelho, E., *Evaluation of bile acid binding capacity of Lactarius deliciosus wild mushrooms polysaccharides and its extracts*, Biophysics Festival, 4th Meeting of Young Biophysicists 4BF, 9-10/05/2024, Covilhã, Portugal. **Poster**
41. Laronha, H., Coreta-Gomes, F., Coimbra, M. A., Coelho, E., *Mushroom polysaccharides: Key players in cholesterol-lowering effect*, XVII Encontro de Química Alimentar, 9-11/10/2024, UTAD, Portugal. **Poster**
42. Machado, F., Gómez-Domínguez, I., Hurtado-Ribeira, R., Martin, D., Coimbra, M. A., del Castillo, M. D., Coreta-Gomes, F., *In vitro digestion of coffee brew and their fractions: their relevance towards cardioprotective*

CQC – Overall Output Indicators 2024

potential, 8th International Conference on Food Digestion (ICFD2024), Porto, Portugal, 9-11/04/2024. **Poster**

43. Oliveira, A. C., Filipe, H. A. L., Gerales, C. F. G. C., Voth, G. A., Moreno, M. J., Loura, L. M. S., *Interaction of MRI Contrast Agent [Gd(DOTA)]⁻ with Lipid Membranes: A Molecular Dynamics Study*, Biophysics Festival, 4th Meeting of Young Biophysicists 4BF, 9-10/05/2024, Covilhã, Portugal. **Poster**

44. Peralta, C., Almeida, Z. C., Lagoa, R., Vaz, D. C., *Protein-ligand interactions: The case of humic acid and laccase*. IMS Open Day, 18th October, Coimbra, Portugal, 2024. **Poster**

45. Peralta, C., Vaz, D.C., Brito, R.M.M., *On the mapping of druggable pockets on the ED domain of Influenza NS1 protein – a review*, Biophysics Festival, 4th Meeting of Young Biophysicists 4BF, 9-10/05/2024, Covilhã, Portugal. **Poster**

46. Silva, S. M., Pires, C. L., Cordeiro, M. M., Moreno, M. J., *Permeation of Weak Acids and Bases Through Vesicles Formed from Cell Membranes*, Biophysics Festival, 4th Meeting of Young Biophysicists 4BF, 9-10/05/2024, Covilhã, Portugal (winner of best poster prize). **Poster**

Conferences / Seminars Organization (35)

1. Valente, Artur J. M., RICI X - 10th Iberian Meeting on Colloids and Interfaces, Coimbra, 23-26 June.2024.
Chairperson
2. Pais, A. A. C. C., RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Scientific Committee
3. Vitorino, C. RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Organizing Committee
4. Antunes, F. RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Organizing Committee
5. Nunes, S. RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Organizing Committee
6. Firmino, T., RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Organizing Committee
7. Pineiro, M. RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Organizing Committee
8. Moreno, M.J. RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Organizing Committee
9. Rosado, M. RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Organizing Committee
10. Marques, Jorge M. C., X Iberian Meeting on Colloids and Interfaces (RICI10), Coimbra, Portugal, 2024, 23-26 June, 2024 **Organizing Committee**
11. Gaspar, J. RICI X - 10th Iberian Meeting on Colloids, Coimbra, Portugal, 23-26 June 2024.
Organizing Committee
12. Valente, Artur J. M. BIOPOL2024 - 9th International Conference on Bio-based and Biodegradable Polymers, Coimbra, Portugal 22-24 July 2024. **Co-chairperson**
13. Murtinho, D. BIOPOL 2024 — 9th International Conference on Bio-based and Biodegradable Polymers, 22–24 July, Coimbra, Portugal, 2024 **Organizing Committee**
14. Ribeiro, Ana CF. BIOPOL 2024 — 9th International Conference on Bio-based and Biodegradable Polymers, 22–24 July, Coimbra, Portugal, 2024 **Organizing Committee**
15. Abreu, P. E. BIOPOL 2024 — 9th International Conference on Bio-based and Biodegradable Polymers, 22–24 July, Coimbra, Portugal, 2024 **Organizing Committee**
16. Gaspar, J. BIOPOL 2024 — 9th International Conference on Bio-based and Biodegradable Polymers, 22–24 July, Coimbra, Portugal, 2024 **Organizing Committee**
17. Valente, Artur J. M., XXVI Congresso SIBAE - Sociedade Ibero-americana de Electroquímica, Lisboa, 19-23.05.10.2024. **National Committee**
18. Pina, João, 22nd International Conference on *Photoacoustic and Photothermal Phenomena* (ICPPP22), Coimbra, Portugal 8-12 July 2024. **Organizing Committee**
19. Sobral, Abilio, Internation Conference in Chemistry – 2024 on Recent Advances in Applied Chemical Sciences, Maulana Azad National Urdu University, Hyderabad, India, 23-24, February, 2024. **International Advisory Board**

CQC – Overall Output Indicators 2024

20. Marques, Jorge M. C., 16° Encontro Nacional de Química Física, Lisbon, Portugal, 2024, 17-19 July 2024. **Organizing Committee**
21. Marques, Jorge M. C., 5° Simpósio de Química Computacional, Lisbon, Portugal, 2024, 17-19 July 2024. **Organizing Committee**
22. C. Serpa, ICPPP22, 22nd International Conference on Photoacoustic and Photothermal Phenomena, Coimbra, Portugal, 8-12 July 2024. **Chair of the Organizing Committee**
23. C. Serpa, ICPPP22 Training School: a hands-on experience, Coimbra, Portugal, 4-5 July 2024. **Chair of the Organizing Committee**
24. Costa, Eduardo. V Congresso SPCAL, 25 e 26 de Janeiro 2024, Faculdade de Medicina - Universidade de Coimbra, Coimbra, Portugal. **Organizing Committee**
25. Pinto, S.M.A., Pereira, M.M., Carrilho, R.M.B., Calvete, M.J.F., S.M.A., *Semifinal das Olimpíadas da Química Júnior- SPQ*, Chemistry Department, University of Coimbra, 2024. **Organizing Committee**
26. Calvete, M.J.F., Pereira, M.M., XII Encontro Nacional de Catálise e Materiais Porosos (XII ENCMP), Coimbra, 6-7 julho de 2024. **Chairperson**
27. Pinho e Melo, T. M. V. D., 29th Congress of the International Society of Heterocyclic Chemistry, (ISHC 2024), 21-26 julho, Aveiro, Portugal, 2024. **Chairperson / President of the International Society of Heterocyclic Chemistry**
28. Soares, M. I. L., 29th Congress of the International Society of Heterocyclic Chemistry (ISHC 2024), 21-26 julho, Aveiro, Portugal, 2024. **Organizing Committee**
29. Burke, A. J., Group for the Promotion of Pharmaceutical chemistry in Academia (GP2A), Auditório da Reitoria, 28-30 agosto, Coimbra, Portugal, 2024. **Scientific Committee**
30. Salvador, A., 2024 Summer School on Computational Biology, 3-13 September 2024, Coimbra, Portugal (Coordinator)
31. Salvador, A. European South Atlantic Biophysics Congress ESAB2024, 4-7 June, San Sebastian, Spain **Scientific and Organizing Committees**
32. Salvador, A. XXII National Congress of Biochemistry, 24-26 October, Aveiro, Portugal **Scientific Committee**
33. Vaz, D. C., I Simpósio em História da Saúde - História em movimento: Uma abordagem interdisciplinar nas ciências da saúde, Escola Superior de Saúde, Instituto Politécnico de Leiria, Leiria, Portugal, 3/05/2024. **Scientific and Organizing Committees**
34. Gaspar, J – SCICOMPT2024 – XII Congresso Nacional de Comunicação de Ciência, Braga, Portugal, 8-10 may 2024 **Scientific Committee**
35. Fangaia, Sónia I. G. XXXIII Reunião Anual de Medicina Dentária e Estomatologia de Coimbra, Março de 2024, Coimbra **Organizing Committee**

Thesis (95)

PhD Thesis (5)

1. Gianluca Utzeri, *Sustainable strategy and bio-based sorbents for pesticides removal*, Universidade de Coimbra, 2024.
[Orientação: Valente, A. J. M.]
2. Daniela N. S. dos Santos, *Unveiling the Excited State Deactivation Mechanisms of Indirubin and Its Role in Metabolic and Oxygen Imaging in Living Cells*, Tese de Doutoramento, 2024.
[Orientação: J. S. Seixas de Melo]
3. Elisa Cristina Marçalo Brás (Chemistry, Molecular Spectroscopy – University of Coimbra, 8 January 2024. *Jet-Cooled and Matrix-Isolated Radicals: Monitoring Interactions and Reactions through IR Spectroscopy*)
[Orientação: Fausto, R. + Cristiano, M. L. S. (University of Algarve, Faro, Portugal) + Shum, M. A. (Max-Planck Institute Göttingen, Germany)]
4. Patrícia Osório Ferreira “*Síntese, caracterização, determinação estrutural e avaliação da solubilidade de formas sólidas multicomponentes dos anti-hipertensivos carvedilol e valsartana*”, Tese de Doutoramento, Universidade Estadual Paulista, Faculdade de Ciências, no Programa de Pós-Graduação em Ciências e Tecnologia de Materiais, Campus de Bauru, 2024.
[Orientação: Caires, F. J., Castro, R. A. E.]
5. Cristiana Lages Pires “*Permeability across distinct cell monolayers as models for BBB: quantitative evaluation of the different permeation routes*”, Tese de Doutoramento, Biological Chemistry, Universidade de Coimbra, 2024.
[Orientação: Moreno, M. J.]

MSc Thesis (37)

1. Maria João Esteves. *Análise Multivariada de Dados Ambientais numa Indústria Vidreira*, Mestrado em Química com especialização em Controlo de Qualidade e Ambiente, Universidade de Coimbra, 2024
[Orientação: S. C.C. Nunes]
2. Ana Raquel Gaspar Sousa Nossa. *Análise Multivariada Dosa Efluentes De Uma Indústria De Pasta De Papel*, Mestrado em Química com especialização em Controlo de Qualidade e Ambiente, Universidade de Coimbra, 2024
[Orientação: T.F. Cova]
3. José António Carvalho Varela, *Deteção e quantificação de iões metálicos libertados de ligas metálicas biomédicas utilizadas*, Mestrado em Medicina Dentária, Área de especialização em Ciências da Saúde, Faculdade de Medicina, Universidade de Coimbra, 2024. [Orientadores: A.C.F. Ribeiro, S.I.G. Fangaia, P. Nicolau].
4. Carolina M. Amaral. *Nanoesponjas de Ciclodextrina contendo Pontos Quânticos de Carbono para a deteção e remoção de Compostos Orgânicos Voláteis*, Mestrado em Química Forense, Universidade de Coimbra, 2024.
[Orientação: Valente, A. J. M.]
5. Cindy Lourenço. *Nanoesponjas de ciclodextrinas para adsorção de fitofármacos*, Mestrado em Química, Universidade de Coimbra, 2024.
[Orientação: Valente, A. J. M.]
6. Ana R. A. Ramos, *Síntese de nanoesponjas à base de amina-ciclodextrina para remoção de antibióticos e corantes sintéticos de soluções aquosas*, Mestrado em Química, Universidade de Coimbra, 2024.
[Orientadores: Murinho, D., Valente, A. J. M.]

CQC – Overall Output Indicators 2024

7. Márcia Alexandra Teixeira Fidalgo, Mestrado em Química, vertente Controlo da Qualidade e Ambiente, *Revalidação do método de quantificação de canabinóides em flor de canábis por RP-HPLC(DAD)*, Tilray (Cantanhede) [Orientação: Jorge Costa Pereira].
8. João Pedro Serodio, projeto de Mestrado em Química, vertente Controlo da Qualidade e Ambiente, *Quantificação de cobalto em fontes de emissão estacionárias de combustão*, CTCV - Centro Tecnológico da Cerâmica e do Vidro (TecnoPolo de Coimbra) [Orientação: Jorge Costa Pereira].
9. S. Nascimento, *Synthesis and Characterization of Polypyrrole/Collagen Composite Scaffolds for Bone Regeneration*, Tese de Mestrado em Engenharia Biomédica, Departamento de Física da Faculdade de Ciências e Tecnologia da Universidade de Coimbra, 2024. [Orientação: Abilio Sobral].
10. L. Russo, *Development of a New Biomaterial Based on Polypyrrole and BODIPYs for Bone Tissue Regeneration*, aluna ERASMUS da Universidade de Pádua, Itália. Tese de Mestrado em Engenharia Biomédica, Departamento de Química da Faculdade de Ciências e Tecnologia da Universidade de Coimbra, 2024. [Orientação: Abilio Sobral].
11. Gabriel Marques, *Desenvolvimento de métodos de deteção seletiva de explosivos através de sondas fluorescentes dispersas em membranas poliméricas*, Mestrado em Química Forense, Universidade de Coimbra, 2024. [Orientação: T. Costa, Co-orientação: J. Sérgio Seixas de Melo]
12. Luís Pedro da Silva Moreira. *Study of the interaction between Abaucin (RS-102895, MLJS-21001) and 7MDX protein using MD*, Mestrado em Biologia Computacional, Universidade de Coimbra, 2024. [Orientação: P. E. Abreu]
13. Ana Rita dos Santos Cunha. *Interação entre Albumina Sérica Humana e Compostos de Interesse Biológico: Cetoprofeno, Ceterolaco e Cafeína*. Universidade de Coimbra, 2024. [Orientação: C. Serpa]
14. João Pedro Antunes Campos. *Avanços na terapia fotodinâmica tópica com um fotossensibilizador de bacterioclorina*. Universidade de Coimbra, 2024. [Orientação: L. G. Arnaut]
15. Lívia Stenico Tanajura. *Mechanisms of cell death activated by photodynamic therapy using a carboxamide halogenated bacteriochlorin named LUZ5*”, University of Coimbra, 2024. [Orientação: L. C. Gomes-da-Silva]
16. António Costa, *Células solares sensibilizadas por corantes pancromáticas*, Universidade de Coimbra, 2024, 2024. [Orientação: C. Serpa]
17. Yonathan Jesus Reis de Andrade. *Funcionalização de fotossensibilizadores para preparação de bioconjugados*, Mestrado em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: Maria Miguéns Pereira e Rafael Tiago Pereira Martins Aroso]
18. Lara Puppini. *Investigation of solid forms of sotagliflozin*, Mestrado em Química e Tecnologia Farmacêutica, Faculdade de Farmácia, Universidade de Bolonha, 2024. [Orientação: Castro, R.A.E.]
19. Filipa Antunes Figueira da Silva. *Investigação do Estado Sólido da Apalutamida*, Mestrado em Química, Departamento de Química, Universidade de Coimbra, 2024. [Orientação: Maria, T. M. R., Castro, R.A.E.]
20. Inês Carolina Ribeiro Pardal, *Investigação de novas formas sólidas do diflunisal*, Mestrado em Química, Departamento de Química, Universidade de Coimbra, 2024. [Orientação: Maria, T. M. R., Castro, R.A.E.]
21. Maria Inês Gomes da Silva, *Investigação de novas formas sólidas de baricitinib*, Mestrado em Química, Departamento de Química, Universidade de Coimbra, 2024.

CQC – Overall Output Indicators 2024

[Orientação: Maria, T. M. R., Canotilho, J.]

22. Marta Susana de Oliveira e Silva Inácio de Sousa. *Relatório de Estágio de Mestrado em Ensino de Física e de Química do 3º ciclo do Ensino Básico e no Ensino Secundário*
Mestrado em Ensino de Física e de Química no 3.º ciclo do Ensino Básico e no Ensino Secundário, Universidade de Coimbra, 2024.

[Orientação: Maria, T. M. R., Alberto, P., Branquinho, A. P.]

23. Maria Miguel Leonor Faria Solano da Rocha, “M090: Mechanism of Binding to Influenza A Virus Hemagglutinin”, *Computational Biology*, University of Coimbra, 2024.

[Orientação: Caridade, P. J. S. B.]

24. Pedro Miguel Mota Sá. *Síntese e Caracterização de Complexos de Corróis para Terapia Fotodinâmica*, Mestrado em Química, Universidade de Coimbra, 2024.

[Orientação: T. M. V. D. Pinho e Melo; Co-orientação: M. Piñero]

25. Catarina Montagril. *Síntese de Compostos Macrocíclicos derivados de Isatina para a doença de Alzheimer*, Mestrado em Química Farmacêutica Industrial, Universidade de Coimbra, 2024.

[Orientação: Anthony Burke]

26. Ricardo Filipe Pereira dos Santos Simões. *Novas Moléculas Pequenas no Combate à Doença de Alzheimer: Histórias de Desenvolvimento e Aplicação*, Mestrado integrado em Ciências Farmacêuticas, Universidade de Coimbra, 2024.

[Orientação: Anthony Burke]

27. Filipa Cardoso. *Drug delivery mediated by macrocyclic compounds for the treatment of Alzheimer 's disease*, Faculty of Pharmacy, University of Coimbra, Mestrado integrado em Ciências Farmacêuticas, Universidade de Coimbra, 2024.

[Orientação: Anthony Burke].

28. Ana Carolina Ramos Quinteiro. *Síntese de Estruturas Orgânicas Porosas para Reações de Catálise Heterogénea*, Mestrado em Química, Universidade de Coimbra, 2024.

[Orientação: D. Murtinho]

29. Pedro Gabriel Simões Gonçalves Miranda. *Hidrogenação por transferência de ácidos resínicos*, Mestrado em Química, Universidade de Coimbra, 2024.

[Co-orientação: D. Murtinho]

30. Cristiana Rodrigues Martins. *Relatório de Estágio de Mestrado em Ensino de Física e de Química no 3.º Ciclo do Ensino Básico e no Ensino Secundário*, Mestrado em Ensino de Física e de Química, Universidade de Coimbra, 2024.

[Orientador Científico de Química: D. Murtinho]

31. Maria Pereira Honório. *Relatório de Estágio de Mestrado em Ensino de Física e de Química no 3.º Ciclo do Ensino Básico e no Ensino Secundário*, Mestrado em Ensino de Física e de Química, Universidade de Coimbra, 2024.

[Orientador Científico de Química: D. Murtinho]

32. Sónia Dias Gomes da Costa. *Relatório de Estágio do Mestrado em Ensino de Física e de Química no 3.º Ciclo do Ensino Básico e no Ensino Secundário*, Mestrado em Ensino de Física e de Química, Universidade de Coimbra, 2024.

[Orientador Científico de Química: M. E. Silva Serra]

33. Beatriz Almeida Melo. *Hidrossililação de Cetonas: Estudos de Otimização*, Mestrado em Química, Universidade de Coimbra, 2024.

[Orientação: M. E. Silva Serra]

34. Catarina Gonçalves. *Análise e caracterização de componentes de colofônia e seus derivados*, Mestrado em Química, Universidade de Coimbra, 2024.

[Orientação: M. Pineiro]

35. Joséia Carla Ferreira Leite de Sousa. *Mecanoquímica e furanos: síntese sustentável de heterociclos*, Mestrado em Química, Universidade de Coimbra, 2024.
[Orientação: A. L. Cardoso; Co-orientação: M. Piñero]

36. Luana Domingues Fonseca. *Estudo da reatividade de furanos e nitroso-alquenos sob ação mecânica*, Mestrado em Química, Universidade de Coimbra, 2024.
[Orientação: M. Piñero; Co-orientação: A. L. Cardoso]

37. Beatriz Barros, *Desenvolvimento de ingredientes alimentares com base em subprodutos de cogumelo *Agaricus bisporus**, Licenciatura em Biotecnologia, Universidade de Aveiro, 2024 [Orientação: Filipe Coreta-Gomes, José António Lopes]

BSc Thesis (53)

1. Ana Wang, *Diagnóstico assistido por computador (CAD): utilização não invasiva de ¹H-NMR para destacar marcadores de cancro em fluidos biológicos*, Estágio Q.Med., Universidade de Coimbra, 2024. [Orientação: J. Costa Pereira]
2. Lara Carolina Antunes dos Santos, *Modelação e previsão da permeabilidade hematoencefálica com ferramentas de inteligência artificial*, Estágio Q.Med., Universidade de Coimbra, 2024. [Orientação: J. Costa Pereira]
3. Beatriz Alves, *FLIM study on the interaction between polyethylenimine (PEI) derivatives with coumarin moities and DNA-like bases*, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: T. Costa, Co-orientação: J. Sérgio Seixas de Melo]
4. Natacha Santos, *FLIM study on the interaction between polyethylenimine (PEI) derivatives with triphenylamine TPA moities and DNA-like bases*, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: T. Costa, Co-orientação: J. Sérgio Seixas de Melo]
5. Beatriz Dias, *Caraterização de sondas fluorescentes à base de pireno para a deteção seletiva de G-quadruplexes*, Licenciatura em Engenharia Biomédica, Universidade de Coimbra, 2024. [Orientação: J. Sérgio Seixas de Melo, Co-orientação: T. Costa]
6. João Cabelo, *Photophysical study on the interaction between polyethylenimine (PEI) derivatives with 7-hydroxy-4-methyl-coumarin and triphenylamine TPA moities and DNA-like bases*, Licenciatura em Engenharia Biomédica, Universidade de Coimbra, 2024. [Orientação: J. Sérgio Seixas de Melo, Co-orientação: T. Costa]
7. Ana Miguel, *Utilização de técnicas computacionais para investigar a interação de pesticidas com proteínas*, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: P. E. Abreu, J. M. C. Marques]
8. Carolina Alexandre, *Utilização de técnicas computacionais para investigar a interação de pesticidas com proteínas*, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: P. E. Abreu, J. M. C. Marques]
9. Maria Martins, *Utilização de técnicas computacionais para investigar a interação da terbutilazina com uma proteína*, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: J. M. C. Marques, P. E. Abreu]
10. Sofia Batista, *Regeneração de Óleos Lubrificantes Usados - Extração supercrítica com dióxido de carbono* Licenciatura em Química, Universidade de Coimbra, 2024 [Orientação: Cecília Santos]
11. Alexandra Casaleiro, *Caracterização das propriedades físico-químicas de óleos lubrificantes - Medidas de TAN e IS*, Licenciatura em Química, Universidade de Coimbra, 2024 [Orientação: Cecília Santos]
12. Ângela S. M. Araújo. *Caracterização de moléculas com interesse farmacêutico através de cálculos de estrutura eletrónica e métodos de aprendizagem computacional*, Licenciatura em Química Medicinal, UC, 2024. [Orientação: S. C.C. Nunes, T.F. Cova]
13. Adriana Casteleiro. *Desenvolvimento de lipossomas ativáveis pela ação da luz a 740 nm*. Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: L. Gomes da Silva]
14. Cláudia Sousa. *Propriedades fotofísicas de complexos bimetálicos de cobre*. Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: C. Serpa]
15. Gabriel Ribeiro. *Fotodegradação de corantes usando nanopartículas de prata suportadas em óxidos metálicos*.

CQC – Overall Output Indicators 2024

Licenciatura em Química. Universidade de Coimbra, 2024.

[Orientação: C. Serpa]

16. Mariana Lebre. *Assessment of the impact of the light wavelength in Photodynamic Therapy in cell culture*

Licenciatura em Química Medicinal, Universidade de Coimbra, 2024.

[Orientação: F. Schaberle]

17. Mariana Lourenço. *Avaliação de novas porfirinas com substituintes sulfonamidas para terapia fotodinâmica*

Licenciatura em Química Medicinal, Universidade de Coimbra, 2024.

[Orientação: L. Gomes da Silva]

18. Matilde Albuquerque. *Viabilidade e Transfecção Fotoacústica de Células COS-7*. Licenciatura em Química Medicinal, Universidade de Coimbra, 2024.

[Orientação: L. Arnaut]

19. Ricardo Rosa. *Desenvolvimento de formulações tópicas para agentes antibacterianos*. Licenciatura em Química Medicinal, Universidade de Coimbra, 2024.

[Orientação: L. Arnaut]

20. Beatriz Ramos Barbosa. *Síntese Sustentável de Amidas via Reação Catalítica de Aminocarbonilação*, Licenciatura em Química, Universidade de Coimbra, 2024 [Orientação: Rui Carrilho; co-orientação: Mário Calvete]

21. João Jordão. *Síntese de fotossensibilizadores para potencial aplicação médica fotodinâmica*, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024 [Orientação: M. J. F. Calvete, R. T. Aroso]

22. Marta Matias. *Estudo Exploratório da Síntese de Nanocristais Farmacêuticos de Diclofenac e Teofilina*, 1º ano, Mestrado em Química, Departamento de Química, Universidade de Coimbra, 2024.

[Orientação: Eusébio, M. E. S.]

23. Gabriela Lopes Morgado. *Formas polimórficas de picolinamida*, Licenciatura em Química, Departamento de Química, Universidade de Coimbra, 2024.

[Orientação: Eusébio, M. E. S.]

24. Marta Susana de Oliveira e Silva Inácio de Sousa. *Determinação da concentração de ferro numa amostra de água por espectrofotometria de absorção molecular no visível – Aplicação de conteúdos de Química abordados no 11º ano - Atividade laboratorial num contexto não formal*, Projeto de Investigação Educacional em Química. Mestrado em Ensino de Física e de Química no 3.º ciclo do Ensino Básico e no Ensino Secundário, Universidade de Coimbra, 2024.

[Orientação: Maria, T. M. R.]

25. Nuno Alexandre da Silva Santos. *Incremento da velocidade de dissolução do diflunisal via co-cristalização com L-prolina*, Licenciatura em Química, Departamento de Química, Universidade de Coimbra, 2024.

[Orientação: Maria, T. M. R., Castro, R.A.E.]

26. Margarida Inês Fernandes Pereira, *Polimorfismo da picolinamida: comportamento térmico do polimorfo II*, Licenciatura em Química, Departamento de Química, Universidade de Coimbra, 2024.

[Orientação: Rosado, M. T. S.]

27. Margarida Rosado Nunes Comenda, *RNA Interferência - uma Classe Inovadora de Medicamentos*, Estágio Curricular, Mestrado Integrado em Ciências Farmacêuticas, Faculdade de Farmácia, Universidade de Coimbra, 2024.

[Orientação: Castro, R.A.E.]

28. Cátia Inês Cardoso Quaresma, *Terapias da Endometriose e a sua relação com a Infertilidade*, Estágio Curricular, Mestrado Integrado em Ciências Farmacêuticas, Faculdade de Farmácia, Universidade de Coimbra, 2024.

[Orientação: Castro, R.A.E.]

CQC – Overall Output Indicators 2024

29. Beatriz Ferreira Almeida, *Hipotiroidismo na gravidez*, Estágio Curricular, Mestrado Integrado em Ciências Farmacêuticas, Faculdade de Farmácia, Universidade de Coimbra, 2024.
[Orientação: Castro, R.A.E.]
30. Vasco José Pereira Fernandes dos Santos, *O estudo do mercado veterinário farmacêutico*, Estágio Curricular, Mestrado Integrado em Ciências Farmacêuticas, Faculdade de Farmácia, Universidade de Coimbra, 2024.
[Orientação: Canotilho, J.]
31. Carina Alexandra Fernandes Coelho, *O papel do farmacêutico na saúde mental*, Estágio Curricular, Mestrado Integrado em Ciências Farmacêuticas, Faculdade de Farmácia, Universidade de Coimbra, 2024.
[Orientação: Canotilho, J.]
32. Mouad Blali, *Toxoplasmose congénita: diagnóstico, tratamento e prevenção*, Estágio Curricular, Mestrado Integrado em Ciências Farmacêuticas, Faculdade de Farmácia, Universidade de Coimbra, 2024.
[Orientação: Canotilho, J.]
33. Ana Sofia Sousa Rosa, “Automated Brain Tumour Segmentation on MRI Using Deep Learning”, Biomedical Engineering - Bioelectronics, Coimbra Institute of Engineering – Polytechnic University of Coimbra, 2024
[Orientação: Caridade, P. J. S. B.]
34. Lia Mariana Pereira Rodrigues Lopes, “Geometrias teóricas de confórmeros de moléculas de antibióticos em modelos de solução e Vácuo”, Medicinal Chemistry, University of Coimbra, 2024.
[Orientação: Caridade, P. J. S. B.]
35. Rodrigo Batista, “Into The Wild: image classification using artificial intelligence”, CTeSP em Instrumentação Biomédica, Coimbra Institute of Engineering - Polytechnic University of Coimbra, 2024.
[Orientação: Caridade, P. J. S. B.]
36. Ricardo Barreira Barreira, “Classificação do estado da doença de Alzheimer através de imagens de RM do cérebro usando inteligência artificial”, CTeSP em Instrumentação Biomédica, Coimbra Institute of Engineering - Polytechnic University of Coimbra,
[Orientação: Caridade, P. J. S. B.]
37. Ricardo Martins Carvalho. *Novel Spiro-β-lactams as Broad-Spectrum Antivirals for RNA Viruses*, Licenciatura em Bioquímica, Universidade de Coimbra, 2024. [Orientação: T. M. V. D. Pinho e Melo; Co-orientação: A. Alves].
38. Andresa Regina Parada Dias. *Síntese em Fluxo Contínuo de Espiro-β-Lactamas com Atividade Biológica*, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: T. M. V. D. Pinho e Melo; Co-orientação: A. Alves]
39. Maria Luísa Crista de Jesus. *Descoberta de Novas Moléculas Vetorizadas para o tratamento da Doença de Alzheimer*, Mestrado Integrado em Química Farmacêutica, Universidade de Coimbra, 2024.
[Orientação: A. Burke]
40. Inês da Silva Martins. *Alterações climáticas e o seu impacto nas doenças infecciosas*, Mestrado Integrado em Ciências Farmacêuticas, Universidade de Coimbra, 2024.
[Orientação: A. M. T. D. P. V. Cabral]
41. Mariana Filipa Liberado Ferraz. *Novos desenvolvimentos no tratamento da Tuberculose*, Mestrado Integrado em Ciências Farmacêuticas, Universidade de Coimbra, 2024.
[Orientação: A. M. T. D. P. V. Cabral]
42. Camila Pombo Alexandre. *Síntese de um polímero orgânico poroso para catálise de reações de Knoevenagel*, Licenciatura em Química, 2024.
[Orientação: D. Murtinho]

43. Maria Tavares Pepino Pereira de Brito. Estudos preliminares da reação de Michael na presença do catalisador R-TAPT-FPB, Licenciatura em Química, 2024. [Orientação: M.E. Silva Serra]
44. Francisco Maria Gaspar Costa e Silva, Estudo da reatividade de furanos e azo-alquenos sob ação mecânica, Licenciatura em Química, 2024. [Orientação: A. L. Cardoso]
45. Gil Guarda Moniz, Mechanochemistry: a way to improve sustainability of furans' transformations, Licenciatura em Bioquímica, 2024. [Orientação: A. L. Cardoso]
46. Joana Margarida Ferreira Vicente. Reação de ésteres alénicos com N-sulfoniliminas catalisada por bases de Lewis, Licenciatura em Química, Universidade de Coimbra, 2024. [Orientação: M. I. Soares]
47. Tiago Portugal dos Santos, 6,7-Bis(Hidroximetil)-1H,3H-Pirrolo[1,2-c]Tiazóis Quirais: Estudo de Novos Agentes Ativadores da p53 para a Terapia do Cancro Colorretal, Licenciatura em Bioquímica, Universidade de Coimbra, 2024. [Orientação: M. I. Soares]
48. Gustavo Filipe M. Mourinho, Estudo da reatividade de alenos com iminas na presença de aminas terciárias, Bolsas Gulbenkian Novos Talentos, Universidade de Coimbra, 2024 (em curso). [Tutoria: M. I. Soares]
49. Beatriz Gomes, *FUNGIACTIV: Propriedades hipocolesterolémicas de compostos extraídos do cogumelo silvestre *Lepista nuda**, Licenciatura em Bioquímica, Universidade de Aveiro, 2024 [Orientação: Filipe Coreta-Gomes, Elisabete Coelho]
50. Catarina Caetano, *Avaliação do potencial hipocolesterolémico de extratos lipídicos da alga *Codium tomentosum**, Licenciatura em Bioquímica, Universidade de Aveiro, 2024 [Orientação: Filipe Coreta-Gomes, Sónia Silva]
51. Daniel F. Santos. *Permeação do Labetalol através de uma Bicamada Lipídica utilizando um Modelo Lipossomal*, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: M. J. Moreno]
52. Madalena B. L. P. Marteleira. *Desenvolvimento de hidrogéis contendo albumina do soro e lipossomas - caracterização das suas propriedades e potencial na ligação e entrega controlada de fármacos*, Licenciatura em Química, Universidade de Coimbra, 2024. [Orientação: M. J. Moreno]
53. Maria A. Reis. Efeito do DMSO na Partição e Permeação do Labetalol em membranas biológicas, Licenciatura em Química Medicinal, Universidade de Coimbra, 2024. [Orientação: M. J. Moreno]

Technical Reports (3)

1. Santos, C. I. A. V., *Relatório Técnico sobre o Método de Regeneração de Óleos Lubrificantes Usados Usando Extração Por Fluido Supercrítico*, Universidade de Coimbra, 2024

2. Carrilho, R.M.B., *CO2PhotoBioPlas - Photosensitive Carbon dioxide-based Polycarbonate Derivatives and Photo-Antimicrobial Polycarbonate-Bioplasticizer Composites*, Relatório Final, Projeto Provas de Conceito 2023 (2024, Universidade de Coimbra e Santander Universities)

3. Caridade, P.J.S.B., “S2CP Final Report”, Cities2030 consortium under the supervision of the project’s coordinator (2024, avaliação do painel da Comissão Europeia).

Lab Prototypes_ Software (1)

1. Caridade, P. J. S. B., Mota, V. C., Galvão, G., Varandas, A. J. C., *Deployment of open-science strategies for potential energy surface at Estudo Gerais repositories* (2024–, GPL license)

Patents (9)

1. *Copolímero Cromogénico, seu Método de Obtenção, Produtos que o Incorporam e Método de Detecção de Contrafação e Autenticação de Produtos.*

Saul Vallejos Calzada, Marta Garcia Gumbre, José Carlos Guirado Moreno, José Miguel Garcia Pérez, Roberto Juan Aguado Garcia, Artur José Monteiro Valente, António Paulo Mendes de Sousa
Patent PT 117491 B (2024/03/07)

2. *Chromogenic copolymer, method of producing the same, products incorporating the same and method for detecting counterfeiting and for products authentication, ChromoSENSOR.*

Saul Vallejos Calzada, Marta Garcia Gumbre, José Carlos Guirado Moreno, José Miguel Garcia Pérez, Roberto Juan Aguado Garcia, Artur José Monteiro Valente, António Paulo Mendes de Sousa
ChromoSENSOR.
European Patent, 21 020 658.7 - 1102 (2024/04/19)

3. *Extracción o separación selectiva de fenoles com polímeros que comprenden grupos borónicos*

José Carlos Guirado Moreno, José Miguel Grcía Pérez, Saúl Vallejos Calzada, Lara González Ceballos, María Teresa Sancho Ortiz, Miguel Angel Fernández Muiño, Sandra María Osés Gómez, Gianluca Utzeri, Artur Valente.
Patent ES2955495 (10/05/2024)

4. *PROCESS FOR THE PRODUCTION OF STARCH BETAINATE*

A.J.M. Valente, P.J.T. Ferreira, D.M.B. Murtinho, R.J. A. Garcia, M. Sharma, A.F.M.
EP4289869A1 (2024.03.27)

5. *A new methodology for Regenerating Waste Lubricant Oils with different properties using Supercritical CO2 Extraction*

Inventores: C.I.A.V. Santos, L.M. Gando Ferreira
Pedido provisório de Patente Portuguesa 20242006567707 (14/10/2024—15:23:53)

6. *Novel Photosensitive Carbon Dioxide Based Polycarbonate Derivatives and Method for Preparation of Photoantimicrobial Polycarbonate-Bioplacitizer Composites and Their Use.*

Inventores: R. M. B. Carrilho, M. M. Pereira, A. C. S. Gonzalez, R. T. P. M. Aroso, G. Piccirillo, F. M. S. Rodrigues.
Pedido de patente PCT internacional, PCT/PT2024/050025 (2024/07/10)

7. Fausto, R., Viegas, L. P., Brito, A. L. B., *Chemometrics Protocol for Semi-Quantitative Analysis of Mixtures Using Spectral Data or Other Composition Dependent Hyper-Redundant Data*, PAT N° 119690. Owners: The authors and the University of Coimbra. Provisory Application: 6 September 2024.

8. *CHLORINE MIT KONDENSIERTEN RINGEN, VERFAHREN UND VERWENDUNGEN DAVON; CHLORINES FUSIONNÉES À UN CYCLE PLATINE (II), PROCÉDÉS ET LEURS UTILISATIONS]*

Inventores: H. D. Burrows, T. M. V. D. Pinho e Melo, A. C. Serra, N. A. M. Pereira, L. M. Martelo, M. Piñeiro Gómez, J. S. S. Melo, J. M. F. P. Batista Pina, M. F. B. R. Botelho, A. M. C. Abrantes, M. Laranjo.
Patente Europeia Concedida EP 3 419 977 (B1), Data de Publicação: 03/01/2024.
Proprietário: Universidade de Coimbra, 3004-531 Coimbra (PT).
Certificado de Efeito Unitário da patente europeia n.º EP 3419977 emitido em 13/02/2024.

9. *Método de produção de papel tissue.*

Inventores: A. C. S. Ferreira, R. J. A. Garcia, D. M. B. Murtinho, A. J. M. Valente, A. M. M. S. Carta, R. A. C. Bértolo, P. C. O. R. Pinto.
Patente portuguesa concedida em 2024.02.23, PT 117053B.

Conference / Journal Proceedings (13)

1. dos Santos, D. N. S., Naskar, N., Reess, K., Delgado-Pinar, E., Seixas de Melo, J. S., Rueck, A., *Metabolic imaging with FLIM/PLIM indirubin derivatives: an ultrafast window into cellular metabolism and oxygen consumption*. In Proceedings Volume 12847, Multiphoton Microscopy in the Biomedical Sciences XXIV, 128470, 2024. <https://doi.org/10.1117/12.3002527>
2. Varela, J., Nicolau, P. M. G., Messias, A., Ribeiro, A. C.F., Valente, A. J. M., Fangaia, S. I. G., *Libertação de iões de cobalto de ligas metálicas biomédicas de Co-Cr, estudo in vitro*, Revista da Sociedade Portuguesa de Estomatologia e Medicina Dentária (SPEMD) Volume65; Supplement - S1, <http://doi.org/10.24873/j.rpemd.2024.12.1328>
3. Seixas de Melo, J. S., *Fast reaction kinetics in the context of cultural heritage*, Lasers and Cultural Heritage, LaserLab Forum, Newsletter of LASERLAB-EUROPE, 37, pp.9, 2024. https://www.laserlab-europe.eu/news-and-press/newsletter-archive/laserlab_nl_37.pdf
4. Raquel C. R. Gonçalves, Sónia C. S. Pinto, J. Pina, Lígia C. Gomes-da-Silva, Susana P. G. Costa, M. Manuela M. Raposo* *“Investigating the Photophysical Properties and Biological Efficacy of BODIPY Derivatives as Photosensitizers in Photodynamic Therapy”*. Chemistry Proceedings. 14, 71, 2023. DOI: <https://DOI.org/10.3390/ecsoc-27-16094>
5. Serrão, G., Scarpelli, F., Rosado, M., Crispini, A., *Quinolines as optimal Halogen-Bonding acceptors*, Acta Crystallogr. A, 80(a1), e537, 2024. DOI: 10.1107/S2053273324094622
6. Chelazzi, L., Ciattini, S., Fantechi, E., Silva, J. F. C., Silva, P. S. P., Silva, M. R., Eusebio, M. E. S., Rosado, M. T. S., *Ranolazine: crystal structure determination and investigation of its metastable polymorphs*, Acta Crystallogr. A, 80(a1):e663, 2024. DOI: 10.1107/S2053273324093367
7. Garcia, T.M.O, Pérez-Parallé, M.L., Rodrigues, S.P.J., *Análise preliminar dos conteúdos relacionados com a água dos Programas dos Ensinos Básico e Secundário de cinco países europeus*. In VII Simposio Internacional de Enseñanza de las Ciencias (SIEC 2024). Vigo, Spain, June 10-13, 2024.
8. Rodrigues, S.P.J., *Química e Literatura: a Ciência está em toda a parte e em todos os tempos*. In SciComPt2024 - Linguagens e Vozes para Uma Ciência Acessível, Santos-Carvalho, Ana, Gerardo, Heloísa, Navalhas, Inês, Ferreira, Miguel (Eds.). Braga, Portugal, May, 8-10, 2024.
9. Peres, M., Rodrigues, S.P.J. *O laboratório químico da Casa Pia de Lisboa: Uma viagem científica no Período Romântico*. In Arte, Cultura e Património do Romantismo. Atas do 3.º Colóquio “Saudade Perpétua”, CEPESE – Centro de Estudos da População, Economia e Sociedade. ISBN: 978-989-8434-50-0 (pp. 440-461).
10. Barreira, R., Caridade, P.J.S.B., Vasconcelos, V., *Classification of Alzheimer’s Disease Stages in MRI Images: A Comparison between VGG19 and ‘Alzheimer Model*, “Computer Vision Applications”. In RECPAD2024, Portuguese Conference on Pattern Recognition (Universidade da Beira Interior, Covilhã, Portugal, 2024).
11. Rosa, S., Caridade, P.J.S.B, Vasconcelos, V, *Evaluating the impact of image filtering on brain tumour segmentation with U-Net*. In RECPAD2024, Portuguese Conference on Pattern Recognition (Universidade da Beira Interior, Covilhã, Portugal, 2024).
12. Burke, A. J., Carreiro, E. P. *Special Edition of Beilstein Journal of Organic Chemistry dedicated to ISySyCat23 - 5th International Symposium on Synthesis and Catalysis (ISySyCat 2023)*, Beilstein J. Org. Chem., 20, 2704–2707, 2024. DOI: 10.3762/bjoc.20.227

13. Pinteus, S., Neves, M., Tecelão, C., Silva, S., Cruz, A., Bernardino, S., Mendes, V., Ribeiro, V., Vaz, D.C., Campos, M.J. *Oxidative Stability of Sunflower Oil Enriched with Fig Tree Leaves Bioactive Compounds at Frying Temperature*. In: Galvão et al., (eds) *Proceedings of the 3rd International Conference on Water Energy Food and Sustainability. ICoWEFS 2023*, pp 145–153. Springer Proceedings in Earth and Environmental Sciences. Springer, Cham, Suíça, 2024.
DOI: 10.1007/978-3-031-48532-9_14

Awards / Distinctions (16)

1. *Triazine porous organic polymers for simultaneous removal and sensing of antibiotics in water*, **Pedro M. C. Matias**, A.C.B. Rodrigues, D. Murtinho, A.J.M. Valente, 16th National Physical Chemistry Meeting, Lisboa, Portugal, 17-19 July, 2024. **Best Oral Communication Award**
2. dos Santos, D. N. S., Naskar, N., Reess, K., Delgado-Pinar, E., Seixas de Melo, J. S., Rueck, A., *Metabolic imaging with FLIM/PLIM indirubin derivatives: an ultrafast window into cellular metabolism and oxygen consumption*, SPIE Photonics West, Moscone Center San Francisco, California, United States, 2024 - **SPIE Student Award**
3. Mafalda Penetra, “*Evaluation of the internalization mechanism of LUZ51*”. European Society for Photobiology Junior Online Meeting, 16 May 2024. **Best Flash Presentation award**
4. Masliy, V., Matos, R., Carrilho, R.M.B., Pereira, M.M., Fernandes, D.M., Peixoto, A.F., *Shrimp shells derived Pd/N-doped biochar for (electro)catalytic applications*, XII ENCMP - XII National Meeting on Catalysis and Porous Materials, Coimbra, Portugal, 2024. **Best Poster Award**
5. Fausto, R., **Appointed as Professor** at the Istanbul Kultur University, Istanbul, Turkey.
6. Fausto, R., Appointed as **ERA-Chair Holder** (*Spectroscopy@IKU – Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals*) (Horizon Europa – Widera 2023 Talents - ERA Chairs Program, Project number: 101184899)
7. Fausto, R., Appointed as **Editor-in-Chief** – Photochemistry and Spectroscopy, SciLight Press, Sydney, Australia.
8. **Baptista, J.A.**, Castro, R.A.E., Fantechi, E., Chelazzi, L., Ciattini, S., Santos, J.C., Marques, J.M.C., Rosado, M.T.S., Eusébio, M.E.S., *New solid-state landscape of an old drug – can structurally related compounds help?*, 2 International Symposium on Chemical Thermodynamics for Young Researchers (ISCTYR), Laurino, Italy, 2024. **Best Oral Communication Award**
9. Fausto, R., **Dedicated Special Issue** of Photochem published: *Photochemistry of Organic Molecules and of Matrix-Isolated Reactive Intermediates: Themed Issue Honoring Professor Rui Fausto for His Contributions to the Field*. DOI: 10.3390/books978-3-7258-2603-2
10. Sérgio P. J. Rodrigues, Associação de Professores da Associação Portuguesa de Professores de Física e Química (APPFQ) **Eleito Membro Honorário em 2024**
11. Silva, S. M., Pires, C. L., Cordeiro, M. M., Moreno, M. J., *Permeation of Weak Acids and Bases Through Vesicles Formed from Cell Membranes*, Biophysics Festival, 4th Meeting of Young Biophysicists 4BF, Covilhã, Portugal 9-10/5/2024. **Prémio de Melhor Poster**
12. Machado, F., Coimbra, M., Coreta-Gomes, F., *Explore cardioprotective potential of coffee and its extracts*, 4th International Conference on Natural Products and Human Health, Aveiro University, 18-20/09/2024. **Best Oral Presentation Honorable Recognition**
13. Laronha, H., Coreta-Gomes, F., Coimbra, M. A., Coelho, E. *Assessment of cholesterol-lowering effects of mushrooms*, XXII National Congress Of Biochemistry, 24-26/10/2024, Aveiro, Portugal **Best Poster Award**
14. *Journal of Medicinal Chemistry* 2024 - **Front Cover Art** (<https://pubs.acs.org/toc/jmcmar/67/24>) - Costa, B. D. P., Simões, J. C. S., Lopes, S. M. M., Laranjo, M., Rodrigues, A. C. B., Gonçalves, A. C., Seixas de Melo, J. S., Botelho, M. F., Pineiro, M., Pinho e Melo, T. M. V. D., *Hydrazone-functionalized trans-A2B-Corroles: Effective Synergy in Photodynamic Therapy of Lung Cancer*, J. Med. Chem., 67, 21934-21951, 2024. DOI: [10.1021/acs.jmedchem.4c01824](https://doi.org/10.1021/acs.jmedchem.4c01824)

CQC – Overall Output Indicators 2024

15. *European Journal of Organic Chemistry* – **Front Cover Picture** (<https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/ejoc.202484201>) - Alves, A. J. S., Silvestre, J. A. D., Pinho e Melo, T. M. V. D., *Continuous Flow Spirocyclization Reactions: Towards Efficient Synthesis of Chiral Spiropenicillanates*, *Eur. J. Org. Chem.*, 27, Art. No. e202400689, 2024.
DOI: [10.1002/ejoc.202400689](https://doi.org/10.1002/ejoc.202400689)

16. Teresa M. V. D. Pinho e Melo na lista “**World’s Top 2% Scientists 2023**” divulgada pelo grupo editorial Elsevier (cientistas mais citados em 2023 e cientistas mais citados ao longo da carreira) [Teresa M. V. D. Pinho e Melo listed in the “World’s Top 2% Scientists 2023” issued by Elsevier].