

Articles in International Peer-Reviewed Journals (181)

1. Chambel, A., Sanati, A. L., Lopes, P. A., Nikitin, T., Fausto, R., de Almeida, A. T., Tavakoli, M., *Laser Writing of Eutectic Gallium–Indium Alloy Graphene-Oxide Electrodes and Semitransparent Conductors*, *Adv. Mater. Technol.*, 7, Art. N. 2101238, 2022.
DOI: 10.1002/admt.202101238
2. Lopes Jesus A. J., Nunes, C. M., Reva, I., *Conformational Structure, Infrared Spectra and Light-Induced Transformations of Thymol Isolated in Noble Gas Cryomatrices*, *Photochem.*, 2, pp. 405–422, 2022.
DOI: 10.3390/photochem2020028
3. Fausto, R., Ildiz, G. O., Nunes, C. M., *IR-induced and Tunneling Reactions in Cryogenic Matrices: The (Incomplete) Story of a Successful Endeavor*, *Chem. Soc. Rev.*, 51, pp. 2853-2872, 2022.
DOI: 10.1039/D1CS01026C
4. Sıdır, İ., Gülseven Sıdır, Y., Góbi, S., Berber, H., Ildiz, G. O., Fausto, R., *UV-Induced –OCH₃ Rotamerization in a Matrix-Isolated Methoxy-Substituted Ortho-Hydroxyaryl Schiff Base*, *Photochem. Photobiol. Sci.*, 21, pp. 835-847, 2022.
DOI: 10.1007/s43630-021-00166-z
5. Sanati, A. L., Chambel, A., Lopes, P. A., Nikitin, T., Fausto, R., Tavakoli, M., *Laser-Assisted Rapid Fabrication of Large Scale Graphene Oxide Transparent Conductors*, *Adv. Mater. Interfaces*, 9, Art. N. 2102343, 2022.
DOI: 10.1002/admi.202102343
6. Nogueira, B. A., Carvalho, M., Paixão, J. A., Eusébio, M. E. S., Lopes, S. M. M., Pinho e Melo, T. M. V. D., Fausto, R., *Portrayal of the Color Polymorphism in the 5-Acetyl-derivative of ROY*, *CrystEngCom*, 24, pp. 1459-1474, 2022.
DOI: 10.1039/d1ce01601f
7. Brito, A. L. B., Brügggen, C., Ildiz, G. O., Fausto, R., *Investigation of Menopause-induced Changes on Hair by Raman Spectroscopy and Chemometrics*, *Spectrochim. Acta A*, 275, Art.N. 121175, 2022.
DOI: 10.1016/j.saa.2022.121175
8. Nunes, C. M., Pereira, N. A. M., Fausto, R., *Photochromism of a Spiropyran in Low-Temperature Matrix. Unprecedented Bidirectional Switching Between a Merocyanine and an Allene Intermediate*, *J. Phys. Chem. A*, 126, pp. 2222-2233, 2022.
DOI: 10.1021/acs.jpca.2c01105
9. Jaleh, B., Hamzehi, S., Sepahvand, R., Azizian, S., Eslamipناه, M., Golbedaghi, R., Meidanchi, A., Fausto, R., *Preparation of Polycarbonate-ZnO Nanocomposite Films: Surface Investigation After UV Irradiation*, *Molecules*, 27, pp. 4448-4461, 2022.
DOI: 10.3390/molecules27144448
10. Nogueira, B. A., Lopes, S. M. M., Pinho e Melo, T. M. V. D., Paixão, J. A., Milani, A., Castiglioni, C., Fausto, R., *Molecular and Crystal Structures of N-Picryl-m-phenolidine and Investigation of Single Crystal Polarized Raman Spectra*, *J. Mol. Struct.*, 1262, Art. N. 133111, 2022.
DOI: 10.1016/j.molstruc.2022.133111
11. Karadag, A., Kaygısız, E., Nikitin, T., Aysal, N., Ildiz, G. O., Fausto, R., *Micro-Raman Spectroscopy and X-ray Diffraction Analyses of the Core and Shell Compartments of an Iron-Rich Fulgurite*, *Molecules*, 27, pp. 3053-3070, 2022.
DOI: 10.3390/molecules27103053
12. Nikitin, T., Lopes, S., Fausto, R., *Matrix Isolation Study of Fumaric and Maleic Acids in Solid Nitrogen*, *J. Phys. Chem. A*, 126, pp. 4392-4412, 2022.
DOI: 10.1021/acs.jpca.2c02770
13. Sıdır, İ., Gultseven Sıdır, Y., Berber, H., Fausto, R., *Solvato-, Thermo- and Photochromism in a New Diazo Diaromatic Dye: 2-(p-Tolyldiazenyl)naphthalen-1-amine*, *J. Mol. Struct.*, 1267, Art. N. 133595, 2022.

DOI: 10.1016/j.molstruc.2022.133595

14. Sidir, İ., Gultseven Sidir, Y., Góbi, S., Berber, H., Fausto, R., *UV-Induced Benzyloxy Rotamerization in a ortho OH-Substituted Aryl Schiff Base*, Photochem, 2, pp. 376-390, 2022.

DOI: 10.3390/photochem2020026

15. Fateixa, S., Nogueira, H. I. S., Paixão, J. A., Fausto, R., Trindade, T., *Insightful Vibrational Imaging Study on the Hydration Mechanism of Carbamazepine*, Phys. Chem. Chem. Phys., 24, pp. 19502-19511, 2022.

DOI: 10.1039/D2CP02185D

16. Brito, A. L. B., Roque, J. P. L., Sidir, İ., Fausto, R., *Low-Temperature Infrared Spectra and UV-Induced Rotamerization of 5-Chlorosalicylaldehyde*, J. Phys. Chem. A, 126, pp. 5148-5159, 2022.

DOI: 10.1021/acs.jpca.2c03685

17. Amado, P. S. M., Lopes Jesus, A. J., Paixão, J. A., Fausto, R., Cristiano, M. L. S., *Unravelling the Structure of Peroxides with Antiparasitic Activity: Relative Impact of a Trioxolane or a Tetraoxane Pharmacophore on the Overall Molecular Structure*, ChemPlusChem, 87, Art. N. e202200207, 2022.

DOI: 10.1002/cplu.202200207

18. Nogueira, B. A., Reart, M., Fausto, R., Castiglioni, C., Dovesi, R., *Raman Activity of the Longitudinal Optical Phonons of the LiNbO3 Crystal. Experimental Determination and Quantum Mechanical Simulation*, J. Raman Spectrosc., 53, pp. 1904-1914, 2022.

DOI: 10.1002/jrs.6426

19. Nunes, C. M., Doddipatla, S., Loureiro, G. F., Roque, J. P. L., Pereira, N. M. A., Pinho e Melo, T. M. V. D., Fausto, R., *Differential Tunneling-driven and Vibrationally-induced Reactivity in Isomeric Benzazirines*, Chem. Eur. J., 28, Art. N. e202202306, 2022.

DOI: 10.1002/chem.202202306

20. Nogueira, B. A., Lopes, S. M. M., Milani, A., André, V., Paixão, J. A., Eusébio, M. E. S., Pinho e Melo, T. M. V. D., Duarte, T., Castiglioni, C., Fausto, F., *Color polymorphs of ROY-ol*, Cryst. Growth Des., 22, pp. 5375-5389, 2022.

DOI: 10.1021/acs.cgd.2c00462

21. Nunes, C. M., Roque, J. P. L., Doddipatla, S., Wood, S. A., McMahon, R. J., Fausto, R., *Simultaneous Tunneling Control in Conformer Specific Reactions*, J. Am. Chem. Soc., 144, pp. 20866-20874, 2022.

DOI: 10.1021/jacs.2c09026

22. Doddipatla, S., Ferreira, G. I., Gülseven Sidir, Y., Nunes, C. M., Fausto, R., *Breaking and Forming of Intramolecular Hydrogen Bonds in Dihydroxybenzaldehydes through UV-induced Conformational Changes in Low-temperature Matrix*, J. Phys. Chem. A, 126, pp. 8645-8657, 2022.

DOI: 10.1021/acs.jpca.2c05839

23. Ivanov, M. S., Nikitin, T., Lopes, S., Xu, J., Duan, Y., Fausto, F., Paixão, J. A., Vilarinho, P. M., Rasing, Th., Semin, S., *Thickness Dependent High-temperature Piezo- and Ferroelectricity in a Fluorenone-based Molecular Crystal*, Adv. Mater. Interfaces, 9, Art. N. 2201103, 2022.

DOI: 10.1002/admi.202201103

24. Lopes Jesus, A. J., Júnior, J. R. L., Fausto, R., Reva, I., *Infrared Spectra and Phototransformations of meta-Fluorophenol Isolated in Argon and Nitrogen Matrices*, Molecules, 27, pp. 8248-8267, 2022.

DOI: 10.3390/molecules27238248

25. Pal, K., Thomas, S., Fausto, R., *Nanoarchitectonics: From Molecules to Advanced Nanomaterials*, J. Mol. Struct., 1270, Art. N. 134003, 2022.

DOI: 10.1016/j.molstruc.2022.134003

26. Costa, T., Knaapila, M., Stewart, B., Ramos, M. L., Justino, L. L. G., Valente, A. J. M., Dalglish, R., Rogers, S. E., Kraft, M., Allard, S., Scherf, U., Burrows, H. D., *Nanostructuring with Surfactants: The Self-Assembly of a New Poly(thiophene-phenylene) Conjugated Polymer Bearing Azacrown Ether Pendant Groups*, Langmuir, 38, pp. 11845-11859, 2022.

DOI: 10.1021/acs.langmuir.2c01246

27. Ildiz, G. O., Tabanez, A. M., Nunes, A., Roque, J. P. L., Justino L. L. G., Ramos, M. L., Fausto, R., *Molecular structure, spectroscopy and photochemistry of alprazolam*, *J. Mol. Struct.*, 1247, Art. N. 131295, 2022.

DOI: 10.1016/j.molstruc.2021.131295

28. Santos, J. A. V., Baptista, J. A., Santos, I. C., Maria, T. M. R., Canotilho, J., Castro, R. A. E., Eusébio, M. E. S., *Pharmaceutical nanocrystal synthesis: a novel grinding approach*, *CrystEngComm* 24, pp 947-961, 2022. “[Magazine cover](#)” – Volume 24, number 5.

DOI: 10.1039/D1CE00407G

29. Gałazkaa, M., Jasiurkowska-Delaporte, M., Eusébio, M.E.S., Rosado, M.T.S., Juszyńska-Gałazka, E., Dryzek, E., *Study on molecular dynamics and phase transitions in 1,2-cyclohexanediol and 1,3-cyclohexanediol isomers by calorimetric and dielectric spectroscopy*, *J. Mol. Liq.*, 2022.

DOI: [10.1016/j.molliq.2022.120874](https://doi.org/10.1016/j.molliq.2022.120874)

30. Cardoso, M. A. Correia, S.F.H.; Goncalves, H.M.R.; Pereira, R.F.P., Maria, T.M.R.; Silva, M.M.; Valente, A.J.M.; Fortunato, E. Ferreira, R.A.S., Rute A. S., Bermudez, V.D., *Solar spectral management with electrochromic devices including PMMA films doped with biluminescent ionosilicas*, *J. Sol-Gel Sci. Technol.*, 101, pp. 58-70, 2022.

DOI: 10.1007/s10971-021-05612-z

31. C. S. Lobo, P. Rodrigues-Santos, D. Pereira, J. Núñez, J. C. D. Trêpa, D. L. Sousa, J. V. Lourenço, M. F. Coelho, L. P. Almeida, J. S. Cunha, L. G. Arnaut, *Photodynamic disinfection of SARS-CoV-2 clinical samples using a methylene blue formulation*, *Photochem. Photobiol. Sci.*, 21, pp 1101-1109, 2022.

DOI: 10.1007/s43630-022-00202-6

32. S. Melo-Guímaro, R. Cardoso, C. João, J. Santos, E. Melro, L. G. Arnaut, J. Pereira, C. Serpa, *Efficient dermal delivery of ascorbic acid 2-glucoside with photoacoustic waves* *Int. J. Cosmetic Sci.*, 44, pp. 453-463, 2022.

DOI: 10.1111/ics.12793

33. R. T. Aroso, L. D. Dias, K. C. Blanco, J. M. Soares, F. Alves, G. J. da Silva, L. G. Arnaut, V. S. Bagnato, M. M. Pereira, *Synergic Dual Phototherapy: Cationic imidazolyl photosensitizers and ciprofloxacin for eradication of in vitro and in vivo E. coli infections*, *J. Photochem. Photobiol. B Biol.*, 233, 112499, 2022.

DOI: [10.1016/j.jphotobiol.2022.112499](https://doi.org/10.1016/j.jphotobiol.2022.112499)

34. C. Donohoe, F. A. Schaberle, F. M. S. Rodrigues, N. Gonçalves, C. J. Kingsbury, M. M. Pereira, M. O. Senge, L. C. Gomes-da-Silva, L. G. Arnaut, *Unravelling the pivotal role of atropisomerism for cellular internalization*, *J. Am. Chem. Soc.*, 144, pp. 15252-15265, 2022.

DOI: [10.1021/jacs.2c05844](https://doi.org/10.1021/jacs.2c05844)

35. R. T. Aroso, G. Piccirillo, L. D. Dias, S. M. A. Pinto, L. G. Arnaut, M. M. Pereira, *Synthesis of Photosensitizers Based On Tetrapyrrolic Macrocycles for Combination with Antibiotics: Dual Inactivation of Bacteria*, *ChemPlusChem*, e202200228, 2022.

DOI: 10.1002/cplu.202200228

36. M. I. P. Mendes, L. G. Arnaut, *Redaporfin Development for Photodynamic Therapy and its Combination with Glycolysis Inhibitors*, *Photochem. Photobiol.*, online, 2022

DOI: 10.1111/php.13770

37. O. A. Chaves, B. A. Iglésias, C. Serpa, *Biophysical Characterization of the Interaction between a Transport Human Plasma Protein and the 5,10,15,20-tetra(pyridine-4-yl)porphyrin*, *Molecules*, 27, 5341, 2022.

DOI: 10.3390/molecules27165341

38. Piotr Gierlich, Luís Rodrigues, Fábio A. Schaberle, Susan Callaghanb, Lígia C. Gomes-da-Silva and Mathias O. Senge *Trimethoxyphenyl-BODIPYs as probes for lysosome staining* *Journal of Porphyrins and Phthalocyanines.*, Vol. 26, No. 08n09, pp. 573-584 (2022)

DOI: 10.1142/S1088424622500328.

39. Claire Donohoe, Stéphanie Leroy-Lhez, Mathias O. Senge, Lígia C. Gomes-da Silva. *POLYTHEA - The opportunities and challenges of doctoral training networks*. Journal of Porphyrins and Phthalocyanines. 2022 April, Vol. 26, No. 08n09, pp. 527-532 (2022)
DOI: 10.1142/S1088424622500250.
40. Schaberle FA, Gomes-da-Silva LC. *A network representation of photodynamic therapy aiming the integration of knowledge and boosting clinical acceptance*. Photodiagnosis Photodyn Ther.;37:102715. March 2022.
DOI: 10.1016/j.pdpdt.2022.102715.
41. Piccirillo, G., Maldonado-Carmona, N., Marques, D. L., Villandier, N., Calliste, C. A., Leroy-Lhez, S., Eusébio, M. E. S., Calvete, M. J. F., Pereira, M. M., *Porphyrin@Lignin nanoparticles: Reusable photocatalysts for effective aqueous degradation of antibiotics*, *Catal. Today*, 2022, em impressão. DOI: 10.1016/j.cattod.2022.09.009
42. Gawne, P. J., Pinto, S. M. A., Nielsen, K. M., Keeling, G. P., Pereira, M.M., Rosales, R. T. M., *Microwave-assisted synthesis of [⁵²Mn]Mn-porphyrins: Applications in cell and liposome radiolabeling*, *Nucl. Med. Biol.*, 114, pp 6, 2022. DOI: 10.1016/j.nucmedbio.2022.08.006.
43. Tomé, V. A., Neves, A. C. B., Pinto, S. M. A., Rodrigues, F. M. S., Calvete, M. J. F., Alves, V. H. P., Sereno, J., Abrunhosa, A. J., Pereira, M. M., *Stable [64Cu]-labelled phthalocyanine choline bioconjugate for development of a potential cancer PET probe. In vivo biodistribution evaluation*, 26, pp 376, 2022. DOI: 10.1142/S1088424622500298.
44. Felgueiras, A. P., Rodrigues, F. M. S., Carrilho, R. M. B., Cruz, P. F., Rodrigues, V. H., Kégl, T. Kollár, L., Pereira, M. M., *Stereoisomeric Tris-BINOL-Menthol Bulky Monophosphites: Synthesis, Characterisation and Application in Rhodium-Catalysed Hydroformylation*, *Molecules*, 27, pp 1989, 2022. DOI: [10.3390/molecules27061989](https://doi.org/10.3390/molecules27061989)
45. Reguero, M., Claver, C., Carrilho, R. M. B., Masdeu-Bultó, A. M., *Immobilized Molecular Catalysts for CO₂ Photoreduction*, *Adv. Sustain. Syst.*, 6, pp 2100493, 2022. DOI: [10.1002/advsu.202100493](https://doi.org/10.1002/advsu.202100493)
46. Alves, L. S., Marques, A. R. A., Padrão, N., Carvalho, F. A., Ramalho, J., Lopes, C., Soares, M. I. L., Futter, C.E., Pinho e Melo, T. M. V. D., Santos, N. C., Vieira, O. V., *Cholesteryl hemiazelate causes lysosome dysfunction impacting vascular smooth muscle cells homeostasis*, *J. Cell. Sci.*, 135, pp jcs254631, 2022.
DOI: 10.1242/jcs.254631
47. Ferreira, M. B., Pereira, N. A. M., Marto, C. M., Cardoso, M., Amaro, I., Coelho, A., Sousa, J., Spagnuolo, G., Ferreira, M. M., Marta Piñeiro, Pinho e Melo, T. M. V. D., Botelho, M. F., Carrilho, E., Paula, A., Laranjo, M., *Isolation and Identification of Cytotoxic Compounds Present in Biomaterial Life®*, *Materials*, 15, pp 871, 2022.
DOI: 10.3390/ma15030871
48. Lopes, S. M. M., Lemos, A., Paixão, J. A., Pinho e Melo, T. M. V. D., *Ethyl 7-acetyl-8a-methyl-3-(1-phenyl-1H-tetrazol-5-yl)-1,4,4a,5,6,8a-hexahydro-7H-pyrano[2,3-c]pyridazine-1-carboxylate*, *Molbank*, M1338, 2022.
DOI: 10.3390/M1338
49. Alves, A. J. S., Alves, N. G., Laranjo, M., Gomes, C. S. B., Gonçalves, A. C., Sarmento-Ribeiro, A. B., Botelho, M. F., Pinho e Melo, T. M. V. D., *Insights into the Anticancer Activity of Chiral Alkylidene-β-Lactams and Alkylidene-γ-Lactams: Synthesis and Biological Investigation*, *Bioorg Med. Chem.*, 63, pp 116738, 2022.
DOI: 10.1016/j.bmc.2022.116738
50. Laranjo, M., Pereira, N. A. M., Oliveira, A. S. R., Aguiar, M. C., Brites, G., Nascimento, B. F. O., B. Serambeque, B., Costa, B. D. P., Pina, J., Seixas de Melo, J. S., Pineiro, M., Botelho, M. F., Pinho e Melo, T. M. V. D., *Ring-fused meso-Tetraarylchlorins as Auspicious PDT Sensitizers: Synthesis, Structural Characterization, Photophysics and Biological Evaluation*, *Front. Chem.*, 10, pp 873245, 2022.
DOI: 10.3389/fchem.2022.873245
51. Barros, G., Serambeque, B., Carvalho, M. J., Marto, C. M., Pineiro, M., Pinho e Melo, T. M. V. D.,

- Botelho, M. F., Laranjo, M., *Applications of photodynamic therapy in endometrial diseases*, *Bioengineering*, 9, pp 226, 2022.
DOI: 10.3390/bioengineering9050226
51. Alves, A. J. S., Alves, N. G., Bártolo, I., Fontinha, D., Caetano, S., Prudêncio, M., Taveira, N., Pinho e Melo, T. M. V. D., *Unveiling a family of spiro- β -lactams with anti-HIV and anti-plasmodial activity via phosphine-catalyzed [3+2] annulation of 6-alkylidene-penicillanates and allenates*, *Front. Chem.*, 10, pp 1017250, 2022.
DOI: 10.3389/fchem.2022.1017250
52. Alves, A. J. S., Silvestre, J. A. D., Pinho e Melo, T. M. V. D., *Synthesis of Novel Chiral Spiro- β -Lactams from Nitrile Oxides and 6-(Z)-(Benzoylmethylene)penicillanate: Batch, Microwave-Induced and Continuous Flow Methodologies*, *RSC Adv.*, 12, pp 30879 – 30891, 2022.
DOI: 10.1039/d2ra04848e
53. Bártolo, I., Moranguinho, I., Gonçalves, P., Diniz, A. R., Borrego, P., Martin, F., Figueiredo, I., Gomes, P., Gonçalves, F., Alves, A. J. S., Alves, N. G., Caixas, U., Pinto, I. V., Barahona, I., Pinho e Melo, T. M. V. D., Taveira, N., *High instantaneous inhibitory potential of bictegravir and the new spiro- β -lactam BSS-730A for HIV-2 isolates from RAL-naïve and RAL-failing patients*, *Int. J. Mol. Sci.*, 23, pp 14300, 2022.
DOI: 10.3390/ijms232214300
54. Ribeiro, J. L. P., Loureiro, J. B., Lopes, S. M. M., Saraiva, L., Pinho e Melo, T. M. V. D., *3-(1,2,3-Triazol-4-yl)- β -Carbolines and 3-(1H-Tetrazol-5-yl)- β -Carbolines: Synthesis and Evaluation as Anticancer Agents*, *Pharmaceuticals*, 15, pp 1510, 2022. [Special issue “State-of-the-art of Medicinal Chemistry in Portugal”]
DOI: 10.3390/ph15121510
55. Pereira, P. A., Serra, M. E. S., Serra, A. C., Coelho, J. F. J., *Application of vinyl polymer-based materials as nucleic acids carriers in cancer therapy*, *Wiley Interdiscip. Rev. Nanomed. Nanobiotechnol.*, 14, pp e1820, 2022.
DOI: 10.1002/wnan.1820
56. Tavares, N. C. T., Cacho, V. R. G., Costa, D. C. S., Nunes, S. C. C., Pais, A. A. C. C., Murtinho, D., Serra, M. E. S., *Deciphering the mechanism behind efficient enantioselective ethylation with thiazolidine-based amino alcohols*, *Appl Organomet Chem*, 36, pp e6567, 2022.
DOI: 10.1002/aoc.6567
57. Machado, T. F., Santos, F. A., Pereira, R. F. P., Bermudez, V. Z., Valente, A. J. M., Serra, M. E. S., Murtinho, D., *β -Ketoenamine Covalent Organic Frameworks—Effects of Functionalization on Pollutant Adsorption*, *Polymers*, 14, pp 3096, 2022.
DOI: 10.3390/polym14153096
58. Ferreira, A. C. S., Aguado, R., Carta, A. M. M. S., Bértolo, R., Murtinho, D., Valente, A. J. M., *Insights into Gum Arabic interactions with cellulose: Strengthening effects on tissue paper*, *Mater. Today Commun.*, 31, pp 103706, 2022.
DOI: 10.1016/j.mtcomm.2022.103706
59. Valente, A. J. M., Pirozzi, D., Cinquegrana, A., Utzeri, G., Murtinho, D., Sannino, F., *Synthesis of β -cyclodextrin-based nanosponges for remediation of 2,4-D polluted waters*, *Environ. Res.*, 215, 114214, 2022.
DOI: 10.1016/j.envres.2022.114214
60. Utzeri, G., Matias, P. M. C., Murtinho, D., Valente, A. J. M., *Cyclodextrin-Based Nanosponges: Overview and Opportunities*, *Front. Chem.*, 10, pp 1–25, 2022.
DOI: 10.3389/fchem.2022.859406
61. Aguado, R., Ferreira, A. C. S., Gramacho, S., Murtinho, D., Valente, A. J. M., *Crosslinking of surface-sizing starch with cyclodextrin units enhances the performance of paper as essential oil carrier*, *Nord Pulp Paper Res J*, 37, pp 413–421, 2022.
DOI: 10.1515/npprj-2022-0034
62. Ferreira, A. C. S., Aguado, R., Carta, A. M. M. S., Bértolo, R., Murtinho, D., Valente, A. J. M., *Influence of DNA as additive for market pulp on tissue paper*, *Nord Pulp Paper Res J*, 37, pp 489–496, 2022.
DOI: 10.1515/npprj-2022-0016

63. Sharma, M., Aguado, R., Murtinho, D., Valente, A.J.M., Ferreira, P.J.T., *Micro-/Nanofibrillated Cellulose-Based Coating Formulations: A Solution for Improving Paper Printing Quality*, *Nanomaterials*, 12, pp 1–18, 2022.
DOI: 10.3390/nano12162853
64. Sharma, M., Aguado, R., Valente, A., Murtinho, D., Ferreira, P., *Dynamic Penetration Profile of Starch Betainate, Pluronic and PCC Coated Papers*, *KnE mater. sci.*, pp 244–250, 2022.
DOI: 10.18502/kms.v7i1.11629
65. Ferreira, A.C.S., Aguado, R., Bértolo, R., Carta, A.M.M.S., Murtinho, D., Valente, A.J.M., *Enhanced water absorption of tissue paper by cross-linking cellulose with poly(vinyl alcohol)*, *Chem. Pap.*, 76, pp 4497–507, 2022.
DOI: 10.1007/s11696-022-02188-y
66. Rénio, M., Murtinho, D., Ventura, M.R., *New bifunctional 1,3-diamine organocatalysts derived from (+)-camphoric acid for asymmetric Michael addition of 1,3-dicarbonyl compounds to nitroolefins*, *Chirality*, 34, pp 782–795, 2022.
DOI: 10.1002/chir.23424
67. Utzeri, G., Murtinho, D., Maria, T.M.R., Pais, A.A.C.C., Sannino, F., Valente, A. J. M., *Amine- β -cyclodextrin-based nanosponges. The role of cyclodextrin amphiphilicity in the imidacloprid uptake*, *Colloids Surf. A Physicochem. Eng. Asp.*, 635, 128044, 2022.
DOI: 10.1016/j.colsurfa.2021.128044
68. Cabral, A. M. T. D. P. V., Fernandes, A. C. G., Joaquim, N. A. M., Veiga, F., Sofio, S. P. C., Paiva, I., Estes, M. A., Rodrigo, M. M., Valente, A. J. M., Ribeiro. A. C. F., *Complexation of 5-Fluorouracil with β -Cyclodextrin and Sodium Dodecyl Sulfate: A Useful Tool for Encapsulating and Removing This Polluting Drug*, *Toxics*, 10, pp 300, 2022.
DOI: 10.3390/toxics10060300
69. Rodrigo, M. M., Valente, A. J. M., Estes, M. A., Cabral, A. M. T. D. P. V., Ribeiro. A. C. F., *Ternary diffusion in aqueous sodium salicylate+sodium dodecyl sulfate solutions*, *J. Chem. Thermodyn.*, 174, pp 106859, 2022.
DOI: 10.1016/j.jct.2022.106859
70. Fangaia, S. I. G., Cabral, A. M. T. D. P. V., Nicolau, P. M. G., Guerra, F. A. D. R. A., Rodrigo, M. M., Ribeiro. A. C. F., Valente, A. J. M., Estes, M. A., *Diffusion of Vanadium Ions in Artificial Saliva and Its Elimination from the Oral Cavity by Pharmacological Compounds Present in Mouthwashes*, *Biomolecules*, 12(7), pp 947, 2022.
DOI: 10.3390/biom12070947
71. Rodrigo, M. M., Cabral, A. M. T. D. P. V., Nicolau, P. M. G., Ribeiro. A. C. F., Valente, A. J. M., Fangaia, S. I. G., Estes, M. A., *Effect of potassium dihydrogen citrate on the diffusion behaviour of citric acid*, *J. Chem. Thermodyn.*, 179, pp 106996, 2022.
DOI: 10.1016/j.jct.2022.106996
Available online: 24 December 2022
72. Brandão, P., Pineiro, M., Burke, A. J., *Tryptanthrin and its derivatives in drug discovery: synthetic insights*, *Synthesis*, 54(19), pp 4235-4245, 2022.
DOI: 10.1055/s-0040-171990
73. Burke, A.J., *Asymmetric organocatalysis in drug discovery and development for active pharmaceutical ingredients*, *Expert Opin Drug Discov*, no prelo, 2022.
DOI: 10.1080/17460441.2023.2160437
74. Carreiro, E.P., Ernesto, S., Gastalho, C., Costa, A. R., Antunes, C. M., Burke, A. J. *Synthesis and Antiproliferative Activity of Novel Quercetin-1,2,3-Triazole Hybrids using the 1,3-Dipolar Cycloaddition (Click) Reaction*, *Synthesis*, 54, pp 4272-4284, 2022.
DOI: 10.1055/s-0040-1719928

75. Amorim, A. C., Fonseca, D. P., Carreiro, E. P., Hermann, G. J., Federsel, H. J., Burke, A. J. *Immobilization of Functionalized epi-Cinchonine Organocatalysts on Controlled Porous Glass-Beads: Applications in Batch and Continuous Flow*, *Synlett*, 33(17), pp 1756-1762, 2022.
DOI: 10.1055/a-1916-4858
76. Soares, M. I. L., Cardoso, A. L., Pinho e Melo, T. M. V. D., *Diels–Alder Cycloaddition Reactions in Sustainable Media*, *Molecules*, 27, pp 1304, 2022.
DOI: 10.3390/molecules27041304
77. Cunha, C., Pinto, A., Galvão, A., Rodríguez, L., Seixas de Melo, J. S., *Aggregation-Induced Emission with Alkynylcoumarin Dinuclear Gold(I) Complexes: Photophysical, Dynamic Light Scattering, and Time-Dependent Density Functional Theory Studies*, *Inorg. Chem.*, 61, 18, 6964–6976, 2022.
DOI: 10.1021/acs.inorgchem.2c00366
78. Delgado-Pinar, E., Pont I., García-España, E., Seixas de Melo, J. S., *Cucurbituril hosts as promoters of aggregation induced emission of triphenylamine derivatives*, *Phys. Chem. Chem. Phys.*, 24, 2403-2411, 2022.
DOI: 10.1039/D1CP04821J
79. Cunha, C., Peixoto, M. S., Santos, J., Abreu, P.E., Paixão, J. A., Pineiro, M., Seixas de Melo, J. S., *Practical Design of 3,6-Di-tert-butylidiphenyldibenzofulvene Derivatives with Enhanced Aggregation-Induced Emission*, *ACS Applied Optical Materials*, 2022.
<https://doi.org/10.1021/acsaom.2c00067>
80. Ferreira, S. C. R., Franchi, M., Pais, A. A. C. C., Seixas de Melo, J. S., *The chemistry behind the first Portuguese postage stamps (1853–1894). A non-destructive analytical and chemometric analysis of pigments, fillers and binders*, *Dyes and Pigments* 205, 110519, 2022.
<https://doi.org/10.1016/j.dyepig.2022.110519>
81. Pinheiro, D., Pineiro, M, Seixas de Melo, J. S., *Tryptanthrin derivatives as efficient singlet oxygen sensitizers*, *Photochem. Photobiol. Sci.* 21, 645-658, 2022.
DOI: 10.1007/s43630-021-00117-8
82. Costa, A. L., Monteiro, R. p., Barradas, P. D. N., Ferreira, S. C. R., Cunha, C., Gomes, A. C., Gonçalves, I. S., Seixas de Melo, J. S., Pillinger, M., *Enhanced thermal and photo-stability of a para-substituted dicumyl ketone intercalated in a layered double hydroxide*, *Front. Chem.*, 10, 2022.
DOI=10.3389/fchem.2022.1004586
83. Pinto, C. M., Pina, J., Delgado-Pinar, E., Seixas de Melo, J. S., *Excited state deactivation mechanisms in Shikonin rationalized from its naphthoquinone parent structures*, *Phys. Chem. Chem. Phys.*, 24, 20348-20356, 2022.
DOI: 10.1039/d2cp01829b
84. Rodrigues, A. C. B., Peixoto, M., Gomes, C., Pineiro, M., Seixas de Melo, J. S., *Aggregation-Induced Emission Leading to White Light Emission in Diphenylbenzofulvene Derivatives*, *Chem. Eur. J.*, 28, e202103768, 2022.
DOI: 10.1002/chem.202103768
85. Ramos, M. L., Justino, L. L. G., Barata, R., Costa, T., Burrows, H. D. *Complexes of In(III) with 8-hydroxyquinoline-5-sulfonate in solution: structural studies and the effect of cationic surfactants on the photophysical behaviour*, *Dalton Trans.* 50, 46, 16970-16983, 2021.
DOI: 10.1039/D1DT02858H.
86. Gonçalves, R. C. R., Belmonte-Reche, E., Pina, J., Costa da Silva, M., Pinto, S. C. S., Gallo, J., Costa Susana, P. G., Raposo, M. M. M., *Bioimaging of Lysosomes with a BODIPY pH-Dependent Fluorescent Probe*, *Molecules*, 27, 8065, 2022.
DOI: 10.3390/molecules27228065
87. Alves, A. A. S., Sousa, F. J. P. M., Sebastiao, M., Antunes, F. E., *Influence of electrolytes on the structural and viscosity properties of mixed anionic–nonionic–zwitterionic surfactants in detergent formulations*, *J. Surfactants Deterg.*, 2022, in press.

DOI: 10.1002/jsde.12613

88. Cordeiro, R., Henriques, M., Silva, J. C., Antunes, F., Alves, N., Moura, C., *Corncob Cellulose Scaffolds: A New Sustainable Temporary Implant for Cartilage Replacement*, *J. Funct. Biomater.*, 13,63,2022.

DOI: 10.3390/jfb13020063

89. Teles, F., Antunes, F., *Novel ranking framework for retrospective simultaneous assessment of fire and mechanical performances of natural fiber-reinforced polymeric composites: Literature update from the previous decade*, *J. Vinyl Addit. Technol.*, 105466, 2022.

DOI: 10.1002/vnl.21908

90. Teles, F., Martins, G., Antunes, F., *Fire retardancy in nanocomposites by using nanomaterial additives*, *J. Anal. Appl. Pyrolysis*, 105466, 2022.

DOI: 10.1016/j.jaap.2022.105466

91. Simões, A. M., Venancio, C., Aves, L., Antunes, F. E., Lopes, L., *Ecotoxicity of cationic cellulose polymers to aquatic biota: The influence of charge density*, *Sci. Total Environ.*, 806, 150560, 2022.

DOI: 10.1016/j.scitotenv.2021.150560

92. Silva, C. V. M., Santos, J. R. C., Rodrigo, M. M., Ribeiro, A. C. F., Valente, A. J. M., Abreu, P. E., Marques, J. M. C., Esteso, M. A., *On the transport and dynamics of disaccharides: H-bonding effect in sucrose and sucralose*, *J. Mol. Liquids*, 345, 117855, 2022.

DOI: 10.1016/j.molliq.2021.117855

93. Fangaia, S. I. G., Nicolau, P. M. G., Guerra, F. A. D. R. A., Rodrigo, M. M., Ribeiro, A. C. F., Valente, A. J. M., Santos, J. R. C., Marques, J. M. C., Esteso, M. A., *The behaviour of aluminium ions in artificial saliva and the impact of the chlorhexidine digluconate on its removal - A diffusion model*, *J. Mol. Liquids*, 353, 118749, 2022.

DOI: 10.1016/j.molliq.2022.118749

94. Vareda, J. P., Matos, P. D., Valente, A. J. M., Durães, L., *A new Schiff base organically modified silica aerogel-like material for metal ions adsorption with Ni selectivity*, *Adsorpt. Sci. Technol*, 8237403, 2022.

DOI: 10.1155/2022/8237403

95. Melro, E., Antunes, F. E., Valente, A. J. M., Duarte, H., Romano, A., Medronho, B., *On the development of phenol-formaldehyde resins using a new type of lignin extracted from pine wood with a levulinic-acid based solvent*, *Molecules*, 27, 2825, 2022.

DOI: 10.3390/molecules27092825

96. Aguado, R., Santos, A. R. M. G., Vallejos, S., Valente, A. J. M., *Paper-based probes with visual response to vapors from nitroaromatic explosives: polyfluorenes and tertiary amines*, *Molecules*, 27, 2900, 2022.

DOI: 10.3390/molecules27092900

97. Arnaiz, A., Guembe-García, M., Delgado-Pinar, E., Valente, A. J. M., Ibeas, S., García, J. M., Vallejos, S., *The role of polymeric chains as a protective environment for improving the stability and efficiency of fluorogenic peptide substrates*, *Scientific Reports*, 12, 8818, 2022.

DOI: 10.1038/s41598-022-12848-4

98. Pereira, J. C., Valente, A. J. M., Söderman, O., α -Cyclodextrin affects the acid-base properties of octanoic acid/sodium octanoate, *J. Mol. Liquids*, 2022, 364, 119955.

DOI: 10.1016/j.molliq.2022.119955

99. Ferreira, B., Sousa, S., Sousa, R. P. C. L., Costa, S. P. G., Raposo, M. M. M., Parpot, P., Valente, A. J. M., Pereira, R. F. P., Figueira, R. B., *Organic-inorganic hybrid sol-gel membranes for pH sensing in highly alkaline environment*, *Constr. Build. Mater.*, 360, 129493, 2022.

DOI: 10.1016/j.conbuildmat.2022.129493

100. Prudente, F. V., Marques, J. M. C., *Thermodynamic Signatures of Structural Transitions and Dissociation of Charged Colloidal Clusters: A Parallel Tempering Monte Carlo Study*, *Molecules*, 27, 2581, 2022.

101. Marques, J. M. C., Prudente, F. V., Pirani, F., *Intermolecular Forces: From Atoms and Molecules to Nanostructures, Molecules*, 27, 2581, 2022.
102. Galindres, D. M., Cifuentes, D., Tinoco, L. E., Murillo-Acevedo, Y., Rodrigo; M. M., Ribeiro, A. C. F., A Review of the Application of Resorcinarenes and SBA-15) in Drug Delivery, *Processes* 10, 4, 684, 2022. DOI: 10.3390/pr10040684
103. Faro, M.P.R. T., Barros, M.C.F., Santos*, C.I.A.V, Ribeiro, A.C.F., *Coupled mutual diffusion in aqueous calcium sulphate + sulphuric acid solutions, J. Chem.Thermodyn.*, 165, 106659, 2022, DOI 10.1016/j.jct.2021.106659
104. Santos, C. I. A. V., Barros, M. C. F., Ribeiro, A.C.F., *Diffusion of Ethanol in Supercritical Carbon Dioxide— Investigation of scCO₂-Cosolvent Mixtures Used in Pharmaceutical Applications, Processes*, 10(4), 660, 2022 DOI 10.3390/pr10040660
105. Santos, C. I. A. V., Barros, M. C. F., Ribeiro, A.C.F., Bou-Ali, M.N., Mialdun, A. _ Shevtsova, V., *Transport properties of n -ethylene glycol aqueous solutions with focus on triethylene glycol-water, J. Chem. Phys.*, 156 (21), 214501, 2022 DOI: 10.1063/5.0091902
106. Santos, C. I. A. V., Barros, M. C. F., Faro, M. P. T. R., Shevtsova, V., Ribeiro, A.C.F., *FTIR as Powerful Tool for Measurements of Diffusion in Supercritical Carbon Dioxide Using Taylor Dispersion Method, Processes*, 10(8), 1528, 2022. DOI:10.3390/pr10081528
107. Romero, C. M., Escamilla, A. P., Ribeiro, A. C. F., Estesó, M. A., *Effect of 1,2-propanediol on the critical micelle concentration of decyltrimethylammonium bromide at temperatures from (293.15 to 308.15) K, Int. J. Mol. Sci.*, 14, 23(24), 15884, 2022. DOI: 10.3390/ijms232415884
108. Ribeiro, A. C. F., Nicolau, P. M. G., Fangaia S. I. G., *Advanced Studies on Drug Delivery Systems: Characterization and its Impact on Pharmaceutical and Medicinal Areas), Processes*, 10, 2427, 2022. DOI: 10.3390/pr10112427
109. Aguirre, A. C., Mauricio Maldonado, Estesó, M. A., *Removal of Toxic Metal Ions Using Poly(BuMA-co-EDMA) Modified with C-Tetra(nonyl)calix[4]resorcinarene, Toxics*, 10, 204, 2022. DOI: 10.3390/toxics10050204
110. Suárez, A. F., Camargo, C. E., Estesó, M. A., Romero, C. M., *Photocatalytic degradation of dielectric mineral oil with PCBs content coupled with algae treatment, Toxics* 10,209, 2022. DOI: 10.3390/toxics10050209
111. Sanabria, E., Estesó, M. A., Edgar F. Vargas, E. F., *Recognition of Heavy Metals by Using Resorcin[4]arenes Soluble in Water, Toxics* 10, 461, 2022. DOI: 10.3390/toxics10080461
112. Estesó, M. A., *Advanced Studies on Toxic Chemicals: Properties and Characteristics, Toxics*, 10, 475, 2022. DOI: 10.3390/toxics10080475
113. Encarnação, T., Mateus, A., Gaspar, F., Santinha, D., Massano, A., Sara Biscaia, S., Guincho, P. B., Nogueira, B. A., Castro, R. E. A., Carvalho, T.A., Eusébio, M. E. S., Fausto, R., Sobral, A. J. F. N., *Bioremediation using microalgae and circular economy approach: a case study, Mater. Proc.*, 108, 8, 2022. DOI:10.3390/materproc2022008108
114. Costa Pereira, J.L.G.F.S., Pais, A. A.C.C., Azevedo, J. C. R., Knapik, H. G., *Methods for unsupervised contribution analysis of raw EEM data in water monitoring. Contaminant identification and quantification, Spect. Acta Part A: Molecular and Biomolecular Spectroscopy*, 264, 120226, 2022. DOI: <https://doi.org/10.1016/j.saa.2021.120226>.

115. Nunes, S.C.C. Nunes, Pais, A.A.C.C., *DNA adsorption on like-charged surfaces mediated by polycations*, *J. Mol. Liq.*, 346, 117060, 2022.
DOI: <https://doi.org/10.1016/j.molliq.2021.117060>.
116. Basso, J.; Mendes, M.; Cova, T.; Sousa, J.; Pais, A.; Fortuna, A.; Vitorino, R.; Vitorino, C. *A Stepwise Framework for the Systematic Development of Lipid Nanoparticles*. *Biomolecules*, 12(2), 223, 2022.
DOI: <https://doi.org/10.3390/biom12020223>.
117. Miranda, M., Veloso, C., Brown, M., Pais, A. A.C. C., Cardoso, C., Vitorino, C., *Topical bioequivalence: Experimental and regulatory considerations following formulation complexity*, *Int. J. Pharm.*, 620, 121705, 2022.
DOI: <https://doi.org/10.1016/j.ijpharm.2022.121705>.
118. Figueiras, A., Domingues, C., Jarak, I., Santos, A.I., Parra, A., Pais, A., Alvarez-Lorenzo, C., Concheiro, A., Kabanov, A., Cabral, H., Veiga, F., *New Advances in Biomedical Application of Polymeric Micelles*, *Pharmaceutics* 14, 1700, 2022.
DOI: <https://doi.org/10.3390/pharmaceutics14081700>
119. Barata, J.F.B., Lacerda, P. S. S., Neves, M. G. P. M. S., Cavaleiro, J. A. S., Ramos, C. I. V., Tomé, A. C., Abreu, P.E., Pais, A. A. C. C., *Reaction of Corroles with Sarcosine and Paraformaldehyde: A New Facet of Corrole Chemistry*, *Int. J. Mol. Sci.* 23, 13581, 2022.
DOI: <https://doi.org/10.3390/ijms232113581>
120. Salazar, I. L., Lourenço, A.S.T., Manadas, B., Baldeiras, I., Ferreira, C., Teixeira, A.C., Mendes, V.M., Novo, A.M., Machado, R., Batista, S., Macário, M.C., Grãos, M., Sousa, L., Saraiva, M. J., Pais, A. A. C.C., Duarte, C. B., *Posttranslational modifications of proteins are key features in the identification of CSF biomarkers of multiple sclerosis*, *Journal of Neuroinflammation*, 2022.
DOI: <https://doi.org/10.1186/s12974-022-02404-2>
121. Veloso C., Videira A.V., Andrade P., Cardoso C., Vitorino C., *In vivo methodologies to assist preclinical development of topical fixed-dose combinations for pain management*, *International Journal of Pharmaceutics*, 2022.
DOI: [10.1016/j.ijpharm.2022.121530](https://doi.org/10.1016/j.ijpharm.2022.121530)
122. Basso J., Paggi M.G., Fortuna A., Vitorino C., Vitorino R., *Deciphering specific miRNAs in brain tumors: a 5-miRNA signature in glioblastoma*, *Molecular Genetics and Genomics*, 2022.
DOI: [10.1007/s00438-022-01866-6](https://doi.org/10.1007/s00438-022-01866-6)
123. Alves L., Ramos A., Rasteiro M.G., Vitorino C., Ferraz E., Ferreira P.J.T., Puertas M.L., Gamelas J.A.F., *Composite Films of Nanofibrillated Cellulose with Sepiolite: Effect of Preparation Strategy*, *Coatings*, 2022
DOI: <https://doi.org/10.3390/coatings12030303>
124. Veloso C., Videira A.V., Andrade P., Cardoso C., Vitorino C., *Topical fixed-dose combinations: Current in vitro methodologies for pre-clinical development*. *International Journal of Pharmaceutics*, 2022.
DOI: [10.1016/j.ijpharm.2022.121621](https://doi.org/10.1016/j.ijpharm.2022.121621)
125. Brites G., Basso J., Miranda M., Neves B.M., Vitorino C., Cruz M.T., *Development of a new hydrogel for the prevention of allergic contact dermatitis*. *International Journal of Pharmaceutics*, 2022.
DOI: [10.1016/j.ijpharm.2022.122265](https://doi.org/10.1016/j.ijpharm.2022.122265)
126. Ferreira N.R., Vitorino C., Fortuna A., *From Antioxidant to Neuromodulator: The Role of Ascorbate in The Management of Major Depression Disorder*, *Biochemical Pharmacology*, 2022
DOI: [10.1016/j.bcp.2022.115300](https://doi.org/10.1016/j.bcp.2022.115300)
127. Zuzarte M., Vitorino C., Salgueiro L., Girão H., *Plant Nanovesicles for Essential Oil Delivery*, *Pharmaceutics*, 2022
DOI: <https://doi.org/10.3390/pharmaceutics14122581>

128. Paulo, V., Pedro, S., Campos, M.G., Delgado, T., Estevinho, L., Anjos, O., *Special bioactivities of phenolics from Acacia dealbata L. with potential for dementia, diabetes and antimicrobial treatments*, *Appl. Sci.* 12(3), 1022, 2022.

DOI: <https://doi.org/10.3390/app12031022>

129. Carreira, L.D., Matias, F.C., Campos, M.G., *Clinical Data on Cannabinoids: Translational Research in the Treatment of Autism Spectrum Disorders*. *Biomedicines* 10, 796, 2022.

DOI: <https://doi.org/10.3390/biomedicines10040796>

130. Santos, M.G., Tietbohl, L., Oliveira, B., Esteves, R., Campos, M.G., Rocha, L., *Phenolic substances and cyanogenesis in galled and non-galled tissue of the fern species *Microgramma vacciniifolia**. *Brazilian Journal of Biology*, 82:1-7; e236151, 2022

DOI: 10.1590/1519-6984.236151

131. Gomes, A., Camara, C., Sousa, A., Santos, F., Campos, M.G., Silva, T., *Chemical composition and free radical-scavenging activities of monofloral bee pollen from *Mimosa pudica* L.*, *Journal of Apicultural Research*, 2022

DOI: 10.1080/00218839.2022.2056290

132. Abbasi, M., Santos, B.P., Pereira, T.C., Sofia, R., Monteiro, N.R.C., Simões, C.J.V., Brito, R.M.M., Ribeiro, B., Oliveira, J.L., Arrais, J.P. *Designing optimized drug candidates with Generative Adversarial Network*, *J. Cheminform.*, 14, 40, 2022.

DOI: 10.1186/s13321-022-00623-6

133. Almeida, Z.L., Brito, R.M.M., *Amyloid Disassembly: What Can We Learn from Chaperones?*, *Biomedicines*, 10, 3276, 2022.

DOI:10.3390/biomedicines10123276

134. Bornes, C., Stosic, D., Geraldes, C.F.G.C., Mintova, S., Rocha, J., Mafra, L., *Elucidating the nature of the external acid sites of ZSM-5 zeolites using NMR probe molecules*, *Chem.Eur. J.* 28, e202201795(1of 6), 2022.

DOI: 10.1002/chem.202201795

135. Botta, M., Geraldes, C.F.G.C., Tei, L., *High Spin Fe(III)-Doped Nanostructures as T₁ MR Imaging Probes*, *WIREs Nanomedicine and Biotechnology*, e1858, 2022.

DOI: 10.1002/wnan.1858

136. Conde-Giménez, M., Galano-Frutos, J.J., Galiana-Cameo, M., Mahía, A., Victor, B.L., Salillas, S., Velázquez-Campoy, A., Brito, R.M.M., Gálvez, J.A., Díaz-de-Villegas, M.D., Sancho, J., *Alchemical Design of Pharmacological Chaperones with Higher Affinity for Phenylalanine Hydroxylase*, *Int. J. Mol. Sci.*, 23, 4502, 2022.

DOI: 10.3390/ijms23094502.

137. Cordeiro, M. M.; Salvador, A.; Moreno, M. J. *Calculation of Permeability Coefficients from Solute Equilibration Dynamics: An Assessment of Various Methods*, *Membranes*, 12, pp 254, 2022.

DOI:10.3390/membranes12030254

138. Ferreira, A.G.M., Santos, J.B., Jalkh, J., Khalighi, S., Cruz, P.F., Brito, R.M.M., *Pressure Effect on the Speed of Sound of Waste Cooking Oil Biodiesel*, *J. Chem. Eng. Data*, 67, pp 3046–3058, 2022.

DOI: 10.1021/acs.jced.2c00473

139. Ferreira, E., Almeida, Z.L., Cruz, P.F., Sousa, M., Verissimo, P., Brito, R.M.M., *Searching for the Best Transthyretin Aggregation Protocol to Study Amyloid Fibril Disruption*, *Int. J. Mol. Sci.*, 23, 391, 2022.

DOI: 10.3390/ijms23010391.

140. Filipe, H. A. L., Loura, L. M. S., *Molecular Dynamics Simulations: Advances and Applications*, *Molecules*, 27, 2105, 2022.

DOI:10.3390/molecules27072105

141. Geraldes, C.F.G.C., Castro, M.M.C. A., Peters, J.A., *Response to Letter to the Editors: “Have we lost an essential link between coordination chemistry and medical applications?”*, *Coord. Chem. Rev.*, 461, 214494, 2022

DOI: 10.1016/j.ccr.2022.2144

142. Geraldes, C.F.G.C., Peters, J.A., *MRI Contrast Agents in Glycobiology*, *Molecules*, 27, 8297, 2022.
DOI: 10.3390/molecules27238297
143. Ledo, A.; Fernandes, E.; Salvador, A.; Laranjinha, J.; Barbosa, R. M. *In vivo hydrogen peroxide diffusivity in brain tissue supports volume signaling activity*. *Redox Biology*, 50, 102250, 2022.
DOI:10.1016/j.redox.2022.102250
144. Lee, H. Y.; Ithnin, A.; Azma, R. Z.; Othman, A.; Salvador, A.; & Cheah, F. C. *Glucose-6-Phosphate Dehydrogenase Deficiency and Neonatal Hyperbilirubinemia: Insights on Pathophysiology, Diagnosis, and Gene Variants in Disease Heterogeneity*. *Frontiers in Pediatrics*, 10, 875877, 2022.
DOI: 10.3389/fped.2022.875877
145. Librando, I. L., Mahmoud, A. G., Carabineiro, S.A.C., Guedes da Silva, M.F.C., Maldonado-Hódar, F.J., Geraldes, C.F.G.C., Pombeiro, A.J.L., *Heterogeneous gold nanoparticle-based catalysts for the synthesis of click-derived triazoles via the azide-alkyne cycloaddition reaction*, *Catalysts*, 12, 45, 2022.
DOI: 10.3390/catal12010045
146. Luís, J.P., Mata, A.I., Simões, C.J.V., Brito, R.M.M., *Conformational Dynamics of the Soluble and Membrane-Bound Forms of Interleukin-1 Receptor Type-1: Insights into Linker Flexibility and Domain Orientation*, *Int. J. Mol. Sci.*, 23, 2599, 2022.
DOI:10.3390/ijms23052599
147. Luís, J.P., Simões, C.J.V., Brito, R.M.M., *The Therapeutic Prospects of Targeting IL-1RI for the Modulation of Neuroinflammation in Central Nervous System Disorders*, *Int. J. Mol. Sci.* 23, 1731, 2022.
DOI:10.3390/ijms23031731
148. Magalhaes, N.; Simões, G. M.; Ramos, C.; Samelo, J.; Oliveira, A. C.; Filipe, H. A. L.; Ramalho, J. P. P.; Moreno, M. J.; Loura, L. M. S. *Interactions between Rhodamine Dyes and Model Membrane Systems—Insights from Molecular Dynamics Simulations*, *Molecules*, 27, 1420, 2022.
DOI:10.3390/molecules27041420
149. Rosário-Ferreira, N.; Bonvin, A. M. J. J.; Moreira, I. S., *Using machine-learning-driven approaches to boost hot-spot's knowledge*, *WIREs Computational Molecular Science*, 2022
DOI: 10.1002/wcms.1602
150. Moreno, M. J.; Loura, L. M. S.; Martins, J.; Salvador, A.; Velazquez-Campoy, A. *Analysis of the Equilibrium Distribution of Ligands in Heterogeneous Media - Approaches and Pitfalls*, *International Journal of Molecular Sciences*, 23, 9757, 2022.
DOI:10.3390/ijms23179757
151. Morfin, J.-F., Lacerda, S., Geraldes, C.F.G.C., Tóth, É., *Metal complexes for the visualisation of amyloid peptides*, *Sensors & Diagnostics*, 1, pp 627–647, 2022.
DOI: 10.1039/D2SD00026A
152. Oliveira, A. C.; Filipe, H. A. L.; Ramalho, J. P. P.; Salvador, A.; Geraldes, C. F. G. C.; Moreno, M. J.; Loura, L. M. S. *Modeling Gd³⁺ Complexes for Molecular Dynamics Simulations: Toward a Rational Optimization of MRI Contrast Agents*, *Inorganic Chemistry*, 61, pp 11837-11858, 2022.
DOI:10.1021/acs.inorgchem.2c01597
153. Pires, C. L.; Silva, I. M. V.; Coimbra, M. A.; Moreno, M. J.; Coreta-Gomes, F. *Effect of Coffee on the Bioavailability of Sterols*, *Foods*, 11, 2935, 2022, DOI:10.3390/foods11192935
154. Primitivo, M. J.; Neves, M.; Pires, C. L.; Cruz, P. F.; Brito, C.; Rodrigues, A. C.; de Carvalho, C. C. C. R.; Mortimer, M. M.; Moreno, M. J.; Brito, R. M. M.; Taylor, E. J.; Millson, S. H.; Reboredo, F.; Jorge Campos, M.; Vaz, D. C.; Ribeiro, V. S. *Edible flowers of Helichrysum italicum: Composition, nutritive value, and bioactivities*, *Food Research International*, 157, 111399, 2022.
DOI:https://doi.org/10.1016/j.foodres.2022.111399

155. Ramos, C. V.; Samelo, J.; Martins, P. A. T.; Moreno, M. J. *Protein Quantification in Complex Matrices*, *J. Chem. Educ.*, 99, pp 1488-1496, 2022.
DOI:10.1021/acs.jchemed.2c00109
156. Sousa, T.; Gouveia, M.; Travasso, R. D. M.; Salvador, A. *How abundant are superoxide and hydrogen peroxide in the vasculature lumen, how far can they reach?* *Redox Biology*, 102527, 2022.
DOI: 10.1016/j.redox.2022.102527
157. Trigueiro-Louro, J., Santos, L.A., Almeida, F., Correia, V., Brito, R.M.M., Rebelo-de-Andrade, H., *NSI protein as a novel anti-influenza target: Map-and-mutate antiviral rationale reveals new putative druggable hot spots with an important role on viral replication*, *Virology*, 565, pp 106-116, 2022.
DOI:10.1016/j.virol.2021.11.001
158. Bueschbell, B; Caniceiro, A. B.; Suzano, P.M.S.; Machuqueiro, M.; Rosário-Ferreira, N.; Moreira, I. S., *Network biology and artificial intelligence drive the understanding of the multidrug resistance phenotype in cancer*. *Drug Resistance Updates* 60, 2022
DOI: 10.1016/j.drug.2022.100811
159. Marques-Pereira, C.; Pires, M. N.; Gouveia, R. P.; Pereira, N. N.; Caniceiro, A. B.; Rosário-Ferreira, N.; Moreira, I.S., *SARS-CoV-2 Membrane Protein: From Genomic Data to Structural New Insights*, *International Journal of Molecular Sciences*, 23 6, 2022
DOI: 10.3390/ijms23062986
160. Sérgio P. J. Rodrigues. *Química e Saúde Pública: Elementos da História de uma relação fundamental*. *Revista Multidisciplinar* 2022
DOI: <https://doi.org/10.23882/rmd.22087>
161. Sérgio P. J. Rodrigues; Pedro J. B. Caridade. *Contributos para a história da química computacional e do uso dos computadores em química*. *História da Ciência e Ensino: construindo interfaces*, 25, 2022, 140-153.
DOI: <http://dx.doi.org/10.23925/2178-2911.2022v25esppl40-153>
162. Paulo Roberto Vilarim, Décio R. Martins, Sérgio P. J. Rodrigues. *Trajectoria e meandros da Educação Escolar Indígena em países colonizados por Espanha*. *ODEERE* 7(3)m 2022, 140-166.
DOI: <https://doi.org/10.22481/odeere.v7i3.11223>
163. Paulo Roberto Vilarim, Décio R. Martins, Sérgio P. J. Rodrigues. *A formação acadêmica como alternativa na divulgação e preservação do etnoconhecimento Terena*. *#Tear Revista de Educação Ciência e Tecnologia* 11(2), 2022.
DOI: <https://doi.org/10.35819/tear.v11.n2.a6201>
164. Paulo Roberto Vilarim, Sérgio P. J. Rodrigues, Décio R. Martins. *Material didático como ferramenta na transmissão do conhecimento tradicional para os professores Terena*. *Intermeio* 28(55), 2022, 194-213.
DOI: <https://doi.org/10.55028/intermeio.v28i55.17296>
165. Paulo Roberto Vilarim, Décio R. Martins, Sérgio P. J. Rodrigues. *Caminhos da Educação Escolar Indígena entre países colonizados pela Inglaterra e suas diferenças*. *ODEERE* 7(2), 2022, 114-135.
DOI: <https://doi.org/10.22481/odeere.v7i2.10860>
166. Vanessa Fonseca, Sérgio P. J. Rodrigues, Maurício Pazinato. *Os currículos dos primeiros cursos de química da universidade de Coimbra e de universidades brasileiras*. *Química Nova*, 2022, no prelo.
DOI: <https://doi.org/10.21577/0100-4042.20170956>
167. Viegas, L. P., *Theoretical Chemistry of Atmospheric Processes*, *Atmosphere*, 13, pp 309, 2022. Editorial.
DOI: 10.3390/atmos13020309
168. Viegas, L. P., *Gas-phase OH-oxidation of 2-Butanethiol: Multiconformer Transition State Theory Rate Constant with Constrained Transition State Randomization*, *Chem. Phys. Lett.*, 803, pp 139289, 2022.
DOI: 10.1016/j.cplett.2022.139829

169. Viegas, L. P., *Atmospheric Degradation of Two Hydrofluoroketones: Theoretical Rate Constants for the Gas-Phase OH-Oxidation of HFK-447mcc and HFK-465mc*, *Atmosphere*, 13, pp 309, 2022.
DOI: 10.3390/atmos13081256

170. Viegas, L. P., *Multiconformer Transition State Theory Rate Constant and Branching Ratios for the OH-Initiated Reaction of CH₃OCF₂CHF₂ and its Primary Product, HC(O)OCF₂CHF₂*, *J. Phys. Org. Chem.*, 2022.
DOI: 10.1002/poc.4470

171. Varandas, A. J. C., *From six to eight P-electron bare rings of group-XIV elements and beyond: can planarity be deciphered from the “quasi-molecules” they embed?*, *Phys. Chem. Chem. Phys.* 4, 8488-8507, 2022.
DOI: 10.1039/d1cp04130d}

172. Mota, V. C., Caridade, P. J. S. B., Varandas, A. J. C. and Galvão, B. R. L., *A quasiclassical-trajectory study of the Si+SH reaction on an accurate DMBE potential energy surface*, *J. Phys. Chem. A*, 126, 3555-3568, 2022.
DOI: 10.1021/acs.jpca.2c01633

173. Pansini, F.N.N., Varandas, A.J.C., *On the continuous solvation model and infrared spectroscopy of liquid water*, *Chem. Phys. Lett.*, 801, 139739, 2022.
DOI: 10.1016/j.cplett.2022.139739

174. Rocha, C. M. R., Linnartz, H., Varandas, A. J. C, *Reconciling spectroscopy with dynamics in global potential energy surfaces: the case of the astrophysically relevant SiC₂*, *J. Chem. Phys.* 157, 104301 2022.

175. Varandas, A. J. C., *Can the quasi-molecule concept help in deciphering planarity? The case of polycyclic aromatic hydrocarbons*, *Int. J. Quantum Chem.* (in press).
DOI: 10.1002/qua.27036

176. Varandas, A. J. C., *Scale-free-modeling (harmonic) vibrational frequencies: Assessing accuracy and cost-effectiveness by CBS extrapolation*, *J. Chem. Phys.* 57, 174110 (2022).
DOI: 10.1063/5.0122268

177. Gregorio, J., Gouveia-Caridade, C. and Caridade, P. J. S. B., *Modeling PM_{2.5} and PM₁₀ Using a Robust Simplified Linear Regression Machine Learning Algorithm*, 13, 1334 (2022).
DOI: 10.3390/atmos13081334

178. Hipólito, N., Martins, S., Ruivo, A., Flora, S., Silva, C.G., Marques, A., Brooks, D., Cruz, J. (2022). *Construct validity and reliability of the Informal Caregiver Burden Assessment Questionnaire (QASCI) in caregivers of patients with COPD*. *Respiratory Medicine* 205: 107027.
DOI: <https://doi.org/10.1016/j.rmed.2022.107027> - Indexado em: Scopus

179. Rama, N., Lages, M., Silva, C.G., Motta Lima, P., Gil, I.C., Guarino, M.P., Oliveira, P., Dixe, M., Rocha, A., Castro-Poças, F., Pimentel, J. (2022). *The Usefulness of Inflammatory Biomarkers to Predict Anastomotic Leakage after Colorectal Surgery: Systematic Review and Meta-Analysis*. *Surg. Gastroenterol. Oncol.*, 27(3): 169-181.
DOI: <https://doi.org/10.21614/sgo-488> - Indexado em: Scopus

180. Rama, N., Lages, M., Guarino, M.P., Lourenço, O., Motta Lima, P., Parente, D., Silva, C.G., Castro, R., Bento, A., Rocha, A., Castro-Poças, F., Pimentel, J. (2022) *Usefulness of serum C-reactive protein and calprotectin for the early detection of colorectal anastomotic leakage: A prospective observational study*. *World J Gastroenterol* 2022, 28(24): 2758-2774.
DOI: <https://doi.org/10.3748/wjg.v28.i24.2758> - Indexado em: Scopus; Web of Science

181. Machado, P., Morgado, M., Raposo, J., Mendes, M., Silva, C.G., Morais, N. (2022). *Effectiveness of exercise training on cancer-related fatigue in colorectal cancer survivors: a systematic review and meta-analysis of randomized controlled trials*. *Support Care Cancer*, 30: 5601–5613.
DOI: <https://doi.org/10.1007/s00520-022-06856-3> - Indexado em: Scopus; Web of Science