

2021

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Thesis / Dissertation

PhD Thesis

Finished

1. RODRIGO, A.P.C. (2021). The biotechnological value of a novel potent marine biotoxin from the polychaete worm *Eulalia viridis*: chemical and toxicological evaluation. Ph.D. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica, 246 pp. Status: Approved. Classification: N/A. FCT grant ref. SFRH/BD/109462/2015
2. Henrique Silva Fernandes Título: Computational studies addressed to PLP-Dependent enzymes Programa Doutoral em Química, FCUP/FEUP, Univ Porto Concluída em Julho de 2021
3. Carla Sílvia Silva Teixeira Título: Computational studies addressed to multifunctional enzyme complexes Programa Doutoral em Química, FCUP/FEUP, Univ Porto Concluída em Julho de 2021
4. Cátia Sofia dos Santos Pereira Novel insights on the interaction of lactoferrin with proton pumping ATPases towards understanding its antifungal and anticancer activities Programa Doutoral em Biologia Molecular e Ambiental Molecular (PDBMA), Univ Minho Concluída em Setembro de 2021
5. RODRIGO, A.P.C. (2021). The biotechnological value of a novel potent marine biotoxin from the polychaete worm *Eulalia viridis*: chemical and toxicological evaluation. Ph.D. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica, 246 pp. Status: Approved. Classification: N/A. FCT grant ref. SFRH/BD/109462/2015
6. Ana Paula Pereira Peixoto Search for new interactions in the top quark sector CERN-THESIS-2021-149.pdf

7. Emanuel Demétrio Mendes Gouveia Universidade do Minho Escola de Ciências Tese de Doutoramento Física Agosto de 2021 Probing the CP nature of the Higgs coupling to top quarks with the ATLAS experiment at the LHC
8. Holography, QCD and Regge Theory Artur Jorge Carvalho Amorim de Sousa (<https://hdl.handle.net/10216/136375>)
9. PhD thesis of Paulo Braz, "Sensitivity to the $0\nu\beta\beta$ decay of ^{136}Xe and development of Machine Learning tools for pulse classification for the LUX-ZEPLIN experiment"

Ongoing

1. GONÇALVES, C. (2019-present). Coleoid venoms: Predicting cephalotoxin function and biotechnological applications from ecological and evolutionary traits. Ph.D. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica. Status: Ongoing. (January 2019). FCT grant ref. SFRH/BD/144914/2019
2. 2021.07128.BD
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4. MARTINS, C. (2017-present). Carcinogenic toxicants and emerging pollutants. A comprehensive case-study on toxicant interactions in vivo and in vitro: from Molecular Toxicology to Environmental Risk Assessment. Ph.D. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica. Status: Ongoing. (September 2017). FCT grant ref. SFRH/BD/120030/2016
5. Inês Raquel Carvalho Leonardo 2020.08210.BD Tecnologias Agrárias e Alimentares Portugal Universidade Nova de Lisboa
6. 2021.07128.BD Rational Development of Nanomedicines for Cardiovascular Diseases.
7. 2020.09087.BD In Silico Optimization of Biocatalysts for Plastic Biodegradation.
8. SFRH/BD/147276/2019 Development of biocidal formulations for effective biofouling control.
9. SFRH/BD/136594/2018 Innovative approach to fight tuberculosis and malaria targeting the extraordinary PLP synthase macromolecular complex.
10. SFRH/BD/137844/2018 New Drugs Against Biofilm Formation and Development: a Computational and Experimental Approach.

Master Thesis

Finished

1. Phytoplankton community in the Algarve coastal region: implications to aquaculture production. MSc Thesis in Ciências do Mar. Universidade de Lisboa
2. CABRAL, I. (2020-present). A computational approach to identify target receptors of marine toxins in the human proteome: Potential biotechnological applications. M.Sc. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica. Status: submitted.
3. SANTOS, M.L. (2021). A transcriptomic approach to the metabolism of porphyrin-like pigments in a marine Polychaeta (*Eulalia* sp.). M.Sc. thesis, Faculdade de Ciências e

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4. GROU, M. (2021). A molecular and pathophysiological approach to tissue regeneration in the planarian model. M.Sc. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica, 40 pp. + Annexes. Final status: Approved. Classification: 19 (0-20).
5. PIMPÃO, A. (2021). Novel developments on the association of the AHR-CYP1A1 axis and arterial hypertension related to obstructive sleep apnea. M.Sc. thesis, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte de Caparica (in collaboration with NOVA Medical School), Universidade Nova de Lisboa, Monte de Caparica, 77 pp. + Annexes. Final status: Approved. Classification: 19 (0-20).
6. Mestrado Informação e Sistemas Empresariais, Univ. Aberta/IST da dissertação intitulada "Feature Selection using LAID and its Implementation on High-Performance Computing Systems" de Paulo Morgado, orientado por L. Cavique e defendido em novembro 2021.
7. P. Xavier and N. Galambaa) Effect of urea on the hydration and aggregation of hydrophobic and amphiphilic solute models: Implications to protein aggregation J. Chem. Phys. 155, 144501 (2021); <https://doi.org/10.1063/5.0064707>
8. Manghnani, K. (2021) Extraction and Visualization of Fake News Indicators (Tese de mestrado) - Instituto Superior Técnico, Universidade de Lisboa. Lisboa, Portugal.
9. Monitorização da população do Roaz-corvineiro (*Tursiops truncatus*) do estuário do Sado. Mestrado em Ecologia e Gestão Ambiental, Universidade de Lisboa, Faculdade de Ciências.
10. "A broad evolutionary perspective of alcoholic fermentation in a non-conventional yeast clade", a ser publicada em Abril 2021 (aluna: Catarina Lagoas)
11. Mestrado Bolonha em Bioengenharia e Nanossistemas, IST/LISBOA "Empowering Antibiotic Polymers Design through Coarse Grained Molecular Dynamics" Gabriel Nascimento Serafim
12. Mariana Luz, Projecto de mestrado com o titulo: "Assessing the Prevalence of Transcription Readthrough in healthy tissues through computational approaches", Mestrado em Genética Molecular e Biomedicina, FCT-NOVA;
13. Valerio Fiori, Projecto de mestrado com o titulo: "Finding Biomarkers of Metastatic Potential in Colorectal Cancer", Mestrado em Bioinformática e Biologia Computacional, FCUL
14. B. Oliveira, "High-Pressure He/H₂/O₂ Mixtures Combustion on the ESTHER Driver: Experiment and Modeling", Ms.C. Thesis, Eng. Aeroespacial, Instituto Superior Técnico, Universidade de Lisboa.
15. Ricardo Silva (2021), Atomic structure calculations in lanthanide ions relevant to kilonovae, FCUL
16. André Cordeiro, Towards the space-time picture of a QCD parton shower, IST
17. Filipa Baltazar (2021), A Monte Carlo based study of the FLASH effect in radiotherapy with protons, IST
18. Miguel Martins, Measurement of the features of muon number distribution using MARTA engineering array, IST
19. Alexandra Fernandes, Measurement of the features of muon number distribution using MARTA engineering array, mestrado em Astronomia e Astrofísica da universidade do Porto

20. Pedro Costa, Detection of astrophysical neutrinos with a gamma-ray observatory, IST
21. Laura Peres, A novel energy reconstruction for high-energy gamma-ray wide field of view observatories, IST
22. Eduardo Ferreira, From light-front wave functions to parton distribution functions, IST MEFT
23. Nuno Fernandes, Development of GPU-Accelerated Trigger Algorithms for the ATLAS Experiment at the LHC, Mestrado em Engenharia Física Tecnológica IST
24. Maria Faria, Investigating the flavour anomalies through the rare beauty decay $B^0 \rightarrow K^* 0 \mu^+ \mu^-$, IST MEFT
25. Beatriz Pinheiro Pereira, Radiation damage of the optical components of the ATLAS TileCal calorimeter at the High-Luminosity LHC, IST MEFT

Conference Paper

1. J. Varela on behalf of the TOFHIR2 design team, TOFHIR2: The readout ASIC of the CMS Barrel MIP Timing Detector, CMS CR-2021/001
2. Anabela Oliveira, Alberto Azevedo, André B. Fortunato, Marta Rodrigues, João Rogeiro, Pedro Lopes, Samuel Bernardo, Jorge Gomes, João Pina, Mario David, 2021 (in press). OPENCoastS: a tailored coastal forecasting WebGIS service, Proceedings of the 3rd Conference of the Arabian Journal of Geosciences, 4 pp.
3. “Plantas ameaçadas de extinção - A Lista Vermelha da Flora Vascular de Portugal Continental”, por André Carapeto (Sociedade Portuguesa de Botânica), a 20 de Janeiro de 2021, integrada nas comemorações do Dia do Município de Vila do Bispo, organizada pela Sociedade Portuguesa de Botânica em parceria com a Câmara Municipal de Vila do Bispo.
4. “A flora ameaçada no Município de Leiria”, por André Carapeto (Sociedade Portuguesa de Botânica), a 25 de Fevereiro de 2021, organizada pela Sociedade Portuguesa de Botânica em parceria com a Câmara Municipal de Leiria e o Centro de Interpretação Ambiental de Leiria.
5. MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. (2021). A study on whole-transcriptomes of two Polychaeta for discovering novel bioproducts with potential biotechnological applications. International Conference for YOUNG Marine Researchers. The Bremen Society for Natural Sciences, Berlin (Germany), September 2021.
6. GONÇALVES, C., MOUTINHO CABRAL, I., RODRIGO, A.P., FONSECA, D., MADEIRA, C., GROSSO, A.R., COSTA, P.M. (2021). A stinging issue: omics and computational tools for the bioprospecting of novel marine toxins. XII European Conference on Marine Natural Products. National University of Ireland, Galway (Ireland), August 2021.
7. MOUTINHO CABRAL, I. (2021). A computational approach to identify target receptors of marine toxins in the human proteome: Potential biotechnological applications. Jornadas Intercalares das Dissertações Anuais dos Mestrados dos Departamentos de Química e Ciências da Vida 2021. NOVA School of Science and Technology, NOVA University of Lisbon, Monte de Caparica (Portugal), February 2021.
8. Deciphering the interaction of lactoferrin with V-ATPase towards a deeper understanding of its mechanisms of action Cátia Santos-Pereira, Juliana F. Rocha, Henrique S. Fernandes,

Lígia R. Rodrigues, Manuela Côrte-Real, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online)

9. Structure-based Virtual Screening, Molecular Dynamics and Free Energy calculations for the identification of novel inhibitors against biofilm formation by *C. violaceum* Fábio G. Martins, André Melo, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online)
10. Structure-based Virtual Screening, Molecular Dynamics and Free Energy calculations for the identification of New Quorum Sensing Inhibitors Fábio G. Martins, André Melo, Sérgio F. Sousa Encontro de jovens investigadores da Universidade do Porto (IJUP) May 7th 2021, Porto, Portugal
11. Specialized multi-level computational approach for the identification of novel quorum sensing inhibitors Fábio G. Martins, André Melo, Sérgio F. Sousa The 24th meeting of the International Society for Molecular Recognition, Affinity 2021 22-24 June 2021, Lisboa, Portugal (online)
12. Identification of potential quorum sensing inhibitors through structure-based virtual screening, molecular dynamics, and free energy calculations Fábio G. Martins, André Melo, Sérgio F. Sousa e-Conference on Innovation in Microbial Control, October 7-8 2021, Porto, Portugal (online)
13. Targeting the PQS system: Discovery of New Quorum Sensing Inhibitors for *P. aeruginosa* through an in silico methodology Tatiana F. Vieira, Rita P. Magalhães, Manuel Simões, Sérgio F. Sousa e-Conference on Innovation in Microbial Control October 7-8, 2021, Porto, Portugal (online)
14. Machine Learning Classification Models for Identification of Ligand-Target Inhibition Pairs in Biofilm Formation in *P. aeruginosa* Rita P. Magalhães, Victor de la Oliva, João Carneiro, Sérgio F. Sousa e-Conference on Innovation in Microbial Control October 7-8, 2021, Porto, Portugal (online)
15. Using Biomolecular Simulations to Understand the Enzymatic Activity of Xanthine Oxidase Henrique S. Fernandes, Sérgio F. Sousa, José J. G. Moura, Luísa B. Maia, Nuno M.F.S.A. Cerqueira BioSeminars@UCIBIO July 21st 2021, Lisbon, Portugal (Online)
16. Exploring the Nitrate and Nitrite Reductase Activity of Xanthine Oxidase – a QM/MM study Henrique S. Fernandes, Sérgio F. Sousa, José J. G. Moura, Luísa B. Maia, Nuno M.F.S.A. Cerqueira 12th Molybdenum and Tungsten Enzymes Conference (MoTEC 2021) September 28th to October 1st 2021, Marseille, France (Online)
17. The Nitrate and Nitrite Reductase Activity of Xanthine Oxidase: a Computational Study Henrique S. Fernandes, Sérgio F. Sousa, José J. G. Moura, Luísa B. Maia, Nuno M.F.S.A. Cerqueira XXI SPB National Congress of Biochemistry October 14th to 16th 2021, Universidade de Évora, Évora, Portugal (Online) Note: Award Best Oral Communication
18. Developed of Inverted Virtual Screening Approaches for the Identification of Protein Targets Associated to the Biological Activity of Specific Molecules Tatiana F. Vieira, Sérgio F. Sousa VIII EJIBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal
19. A multidisciplinary approach to untangle the mechanisms behind the antifungal activity of lactoferrin Cátia Santos-Pereira, María T. Andrés, Juliana F. Rocha, Henrique S. Fernandes, Susana R. Chaves, José F. Fierro, Hernâni Gerós, Stéphen Manon, Sérgio F. Sousa, Lígia R.

- Rodrigues, Manuela Côrte-Real 15th International Conference on Lactoferrin: Structure, Function and Applications December 6-10th 2021, Beijing, China (online)
20. Multilocus DNA metabarcoding of complex mixtures containing members of the Boraginaceae family: a step further to assure food safety and quality Inês CARVALHO LEONARDO, Martijn STAATS, Marleen VOORHUIJZEN, Valerie VAN DER VORST, Bas FRONEN, Jorge CAPELO, Maria Teresa BARRETO CRESPO, Frédéric BUSTOS GASPAR November 2021 ISEKI e-conference 2021 - Food Texture, Quality, Safety and Biosecurity in the Global Bioeconomy Online (Austria)
 21. Multilocus DNA metabarcoding of complex mixtures containing members of the Boraginaceae family for food safety and quality assurance Inês Carvalho Leonardo, Martijn Staats, Marleen Voorhuijzen, Valerie van der Vorst, Bas Fronen, Jorge Capelo, Maria Teresa Barreto Crespo, and Frédéric Bustos Gaspar November 2021 Microbiotec'21 - Congress of Microbiology and Biotechnology 2021
 22. Two-particle Correlations in multi-Regge Kinematics, N. B. de Leon, G. Chachamis and A. S. Vera, arXiv:2112.13794 [hep-ph]; contribution to Low-x workshop 2021
 23. New results on the modification of jet structure in Heavy Ion collisions, Helena Santos, on behalf of the ATLAS, ALICE and CMS Collaborations, PoS(LHCP2021)082, <https://doi.org/10.22323/1.397.0082>
 24. Rare heavy-flavour decays, A. Boletti (on behalf of the ATLAS, CMS, and LHCb Collaborations), PoS(LHCP2021)139
 25. Comparison of Voxel S-values and Monte Carlo Simulation in [¹⁷⁷Lu]Lu-DOTA-TATE Quantification for Patient-Specific Dosimetry, Rodrigues, C., Ferreira, P., Oliveira, F. P. M., Silva, Â., Peralta, L., Costa, D. C., Eur J Nucl Med Mol Imaging, 48 (2021) S75, <https://doi.org/10.1007/s00259-021-05547-1>
 26. Study of central exclusive production of top quark-antiquark pairs at LHC, M. Pisano, Nuovo Cimento 44C (2021) 66
 27. Gamma/hadron discrimination using a small-WCD with four PMTs, R. Conceição, P. Assis, F. Assunção, A. Bakalova, U. Barres de Almeida, C. Roque Bom, J. Correia, A. De Angelis, L.O. Dias, B. Serrano González, A. Guillén, G. La Mura, N. Lourenço, P. Machado, S. Marques, L. Mendes, M. Pimenta, R. Shellard, B. Tomé and J. Vicha, Proceedings of 37th International Cosmic Ray Conference - PoS(ICRC2021) 395(2021) 707, <https://doi.org/10.22323/1.395.0707>
 28. Monitoring Gamma-Ray Burst VHE emission with the Southern Wide-field-of-view Gamma-ray Observatory, G. La Mura, Proceedings of 37th International Cosmic Ray Conference - PoS(ICRC2021) 395(2021) 709, <https://doi.org/10.22323/1.395.0709>
 29. New methods to reconstruct Xmax and the energy of gamma-ray air showers with high accuracy in large wide-field observatories, R. Conceição, L. Peres, M. Pimenta and B. Tomé, Proceedings of 37th International Cosmic Ray Conference - PoS(ICRC2021) 395(2021) 711, <https://doi.org/10.22323/1.395.0711>
 30. Search for new physics in $b \rightarrow s\ell + \ell^-$ transitions at CMS, A. Boletti, on behalf of the CMS Collaboration, PoS(ICHEP2020)365
 31. The ATLAS Hardware Track Trigger performance studies for the HL-LHC, A. L. Moreira de Carvalho on behalf of the ATLAS Collaboration, PoS(LHCP2020)247
 32. Jet substructure modification probes the QGP resolution length, J. Casalderrey-Solana, G. Milhano, D. Pablos and K. Rajagopal, Nucl.Phys.A 1005 (2021) 121904,

10.1016/j.nuclphysa.2020.121904

33. Impact of LHC jet data on Parton Distribution Functions, João Pires, PoS LHCP2020 (2020) 145, 10.22323/1.382.0145
34. Gamma-ray Astrophysics in the MeV Range The ASTROGAM Concept and Beyond, A. De Angelis, V. Tatischeff, S. Brandt, A. Bulgarelli, R. Curado da Silva, I. Grenier, L. Hanlon, D. H. Hartmann, M. Hernanz, G. Kanbach, I. Kuvvetli, P. Laurent, M. Mariotti, M. N. Mazziotta, J. Mc Enery, A. Morselli, K. Nakazawa, M. Pearce, J. Rico, X. Wu, S. Zane, A. Zoglauer, Exp. Astron. 51 (2021) 1225-1254, 10.1007/s10686-021-09706-y

Conference Poster

1. RODRIGO, A.P., GROSSO, A., MENDES, V.M., MANADAS, B., BATISTA, P.V., FERNANDES, A.R., COSTA, P.M. (2021). Unveiling venomous annelids by combining omics with ecological traits: The example of a phyllodocid. 12th European Conference on Marine Natural Products, Galway (Ireland), September 2021.
2. Borges V. 2021 (23 March). Título: "INSaFLU: open web-based bioinformatics suite for genome-based surveillance of influenza virus and other pathogens, such as SARS-CoV-2"; Encontro: Joint ECDC-WHO EURO virus characterisation working group meeting, World Health Organization (WHO) and European Centre for Disease Prevention and Control (ECDC)
3. MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. (2021). A study on whole-transcriptomes of two Polychaeta for discovering novel bioproducts with potential biotechnological applications. International Conference for YOUNG Marine Researchers. The Bremen Society for Natural Sciences, Berlin (Germany), September 2021.
4. Integrated biochemical and computational approach reveals novel mechanisms underlying the antifungal activity of the milk-derived lactoferrin protein Cátia Santos-Pereira, María T. Andrés, Juliana F. Rocha, Henrique S. Fernandes, Susana R. Chaves, José F. Fierro, Hernâni Gerós, Stéphen Manon, Sérgio F. Sousa, Lígia R. Rodrigues, Manuela Côrte-Real XXI SPB National Congress of Biochemistry 14-16th Oct 2021, Évora, Portugal (online)
5. Application of QM/MM methods for development of plastic degradation enzymes Jorge M. Cunha, Rita P. Magalhães, Henrique S. Fernandes, Sérgio F. Sousa Encontro de jovens investigadores da Universidade do Porto (IJUP) May 6th 2021, Porto, Portugal (online)
6. Integrated in silico approach for the development of a new antipsychotic drug candidate to treat schizophrenia Rodrigo Andrade, Elina Marinho, Alba Iglesias, Jose Brea, Marián Castro, Filipe A. Almeida Paz, Filipe M. Areias, Maria I. Loza, Sérgio F. Sousa and M. Fernanda Proença Encontro de jovens investigadores da Universidade do Porto (IJUP) May 7th 2021, Porto, Portugal
7. Borges V. 2021. (23 March). Título: "Add-value of SARS-CoV-2 minor variant analysis: some practical examples". I-MOVE-COVID-19 annual meeting.
8. Development of a Structural Database of Insecticide Targets Maria F. Araújo, Tatiana F. Vieira, Elisabete M.S. Castanheira Coutinho and Sérgio F. Sousa Encontro de jovens investigadores da Universidade do Porto (IJUP), May 7th 2021, Porto, Portugal

9. Molecular Docking, Molecular Dynamics, and Free Energy Calculations for Identification of New Drugs Against Biofilm Formation in *P.aeruginosa* Rita P. Magalhães, Tatiana F. Vieira, André Melo, Sérgio F. Sousa Hünfeldt 2021: Workshop on Computer Simulation and Theory of Macromolecules April 23-24 2021 (online)
10. Identification of Biofilm Formation Inhibitors in *Pseudomonas aeruginosa* through Virtual Screening, Molecular Dynamics, and Free Energy Calculations Rita P. Magalhães, Tatiana F. Vieira, André Melo, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online) Best Poster Communication
11. Bioinformatic applications for the development of plastic degradation enzymes using QM/MM Jorge M. Cunha, Rita P. Magalhães, Henrique S. Fernandes, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online)
12. Development of a Structural Database of Insecticide Targets Maria F. Araújo, Tatiana F. Vieira, Elisabete M.S. Castanheira Coutinho, Sérgio F. Sousa X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online)
13. 3D Prediction of Non-B DNA Conformations Associated with MtDNA Genomic Instability André F. Pina, Sérgio F. Sousa, João Carneiro X Bioinformatics Open Days May 6th 2021, Braga, Portugal (online)
14. In silico methodology for the identification of new drugs against biofilm formation in *P. aeruginosa* Tatiana F. Vieira, Rita P. Magalhães, Sérgio F. Sousa Affinity 2021: The 24th meeting of the International Society for Molecular Recognition 22-24 June 2021 (online)
15. Discovery of New Drugs Against Biofilm Formation in *P.aeruginosa* through Molecular Docking, Virtual Screening, Molecular Dynamics and MM/GBSA calculations Rita P. Magalhães, Tatiana F. Vieira, André Melo, Sérgio F. Sousa Affinity 2021: The 24th meeting of the International Society for Molecular Recognition 22-24 June 2021 (online)
16. Elucidating the interaction of lactoferrin with V-ATPase towards understanding its mechanisms of action Cátia Santos-Pereira, Juliana F. Rocha, Henrique S. Fernandes, Lígia R. Rodrigues, Manuela Côrte-Real, Sérgio F. Sousa. The 24th meeting of the International Society for Molecular Recognition, Affinity 2021, 22-24 June 2021 Note: Young investigator award
17. A Multi-Level Computational Approach in the Discovery of New Quorum Sensing Inhibitors for *P. aeruginosa* Tatiana F. Vieira , Cristina Sousa, Sérgio F. Sousa Paul Ehrlich (PE) Euro-PhD Network virtual meeting, MedChem2021 26-28 July 2021 (online)
18. Development of a Classification Model for the Identification of Targets to Known *P.aeruginosa* Biofilm Formation Inhibitors Rita P. Magalhães, Victor de la Oliva, João Carneiro, Sérgio F. Sousa Machine Learning in Quantum Physics and Chemistry Summer School 24 August to 3 September 2021, Warsaw, Poland Note: Award for 3rd Best Poster
19. Specialized Multi-Level Computational Approach For The Identification of Novel Quorum Sensing Inhibitors Fábio G. Martins, André Melo, Sérgio F. Sousa EMBO virtual Workshop Advances and challenges in biomolecular simulations 18-21 October 2021, Bioexcel (online)
20. Optimization of a Drug Discovery Computer Aided Workflow for Identification of *P.aeruginosa* Quorum-Sensing Inhibitors Rita P. Magalhães, Tatiana F. Vieira, André Melo, Sérgio F. Sousa EMBO virtual Workshop Advances and challenges in biomolecular simulations 18-21 October 2021, Bioexcel (online)

21. The catalytic mechanism of Nitrilase 2: the role of the Cys-Glu-Lys catalytic triad Carla S. Silva Teixeira, Nuno M.F.S.A. Cerqueira, Sérgio F. Sousa 18th European Symposium on Organic Reactivity (ESOR2021) 21-23 September 2021, Vrije Universiteit Amsterdam, The Netherlands (online)
22. The Cys-Glu-Lys catalytic triad from the nitrilase superfamily: a QM/MM study on Nitrilase 2 Carla S. Silva Teixeira, Nuno M.F.S.A. Cerqueira, Sérgio F. Sousa EMBO virtual Workshop Advances and challenges in biomolecular simulations 18-21 October 2021, Bioexel (virtual)
23. Unveiling the catalytic mechanism of the Cys-Glu-Lys catalytic triads using the Nitrilase 2 as a case study Carla S. Silva Teixeira, Nuno M.F.S.A. Cerqueira, Sérgio F. Sousa VIII EJBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) 7December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal
24. Unraveling the Catalytic Mechanism of Threonine Aldolase, a potential biocatalyst for industrial application Juliana F. Rocha, Sérgio F. Sousa, Nuno M. F. S. A. Cerqueira FEBS 2021 Advanced Course - Computational Approaches to Understanding and Engineering Enzyme Catalysis October 19-22st 2021, Oulu, Finland (online) - Flash Talk
25. The Catalytic Mechanism of the SARS-Cov-2 Main Protease Henrique S. Fernandes, Sérgio F. Sousa, Nuno M.F.S.A. Cerqueira VIII EJBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal
26. Optimization of Classification Models for Identification of Ligand-Target Inhibition Pairs in Biofilm Formation in *P.aeruginosa* Rita P. Magalhães, Victor de la Oliva, João Carneiro, Sérgio F. Sousa VIII EJBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal
27. A computational study on the catalytic mechanism of Pdx2: a glutaminase containing the Cys-His-Glu triad André F. Pina, Sérgio F. Sousa, Nuno M.F.S.A. Cerqueira VIII EJBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal
28. Specialized Multi-Level Computational Protocol for the Identification of Potential New Drugs Fábio G. Martins, Tatiana F. Vieira, Joel P. Moreira, Tiago Barbosa, Sérgio F. Sousa VIII EJBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal
29. Unraveling the catalytic mechanism of Threonine aldolase - a critical enzyme in the pharmaceutical industry Juliana F. Rocha, Sérgio F. Sousa, Nuno M.F.S.A. Cerqueira VIII EJBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal
30. Bridging the gap between lactoferrin and V-ATPase through a multi-stage computational approach Cátia Santos-Pereira, Juliana F. Rocha, Henrique S. Fernandes, Lígia R. Rodrigues, Manuela Côrte-Real, Sérgio F. Sousa VIII EJBCE (Encontro de Jovens Investigadores de Biologia Computacional Estrutural) December 21st 2021, Faculdade de Ciências e Tecnologia da Universidade de Coimbra, Coimbra, Portugal

31. Molecular detection of species from the Boraginaceae family to safeguard food and feed safety, integrity, authenticity, and quality Inês Carvalho Leonardo, Jorge Capelo, Maria Teresa Barreto Crespo, and Frédéric Bustos Gaspar November 2021 Microbiotec'21 - Congress of Microbiology and Biotechnology 2021
32. The complete genome sequence of *Alicyclobacillus acidoterrestris* DSM 3922T, a food spoiler taint producing strain Inês Carvalho Leonardo, Maria Teresa Barreto Crespo, and Frédéric Bustos Gaspar November 2021 Microbiotec'21 - Congress of Microbiology and Biotechnology 2021
33. Adaptation of SPARK to atmospheric-pressure micro-plasma jet flow conditions Duarte Gonçalves, João Santos Sousa, Stéphane Pasquiers, Mário Lino da Silva, Luís Lemos Alves PLATHINIUM 2021
34. Sinval, J.; Vazquez, A.C.S.; Hutz, C.S.; Schaufeli, W.B.; Silva, S. Burnout Assessment Tool (BAT): Validity Evidence from Brazil and Portugal. *Int. J. Environ. Res. Public Health* 2022, 19, 1344. <https://doi.org/10.3390/ijerph19031344>
35. Collective dynamics of heavy ion collisions in ATLAS, Helena Santos, on behalf of the ATLAS Collaborations, ISMD2021 - International symposium on multiparticle dynamics
36. Collective dynamics of heavy ion collisions in ATLAS, Helena Santos, on behalf of the ATLAS Collaboration, 50th International Symposium on Multiparticle Dynamics
37. Evidence for local acceleration of heavy >10 MeV/n oxygen and sulphur in Jupiter's innermost radiation belts, Elias Roussos, Christina Cohen, Peter Kollmann, Marco Pinto, Patricia Gonçalves, Norbert Krupp, and Konstantinos Dialynas, Europlanet Science Congress 2021, <https://doi.org/10.5194/epsc2021-603>
38. Gamma/hadron discrimination using a small-WCD with four PMTs, R. Conceição et al., for the SWGO collaboration, 37th International Cosmic Ray Conference (Berlin)
39. Modeling the radiobiological effects of gold nanoparticles in proton therapy of glioblastomas, J. Antunes, F. Mendes, A. Paulo and J. M. Sampaio, PANIC 2021, Particles and Nuclei International Conference
40. Monitoring Gamma-Ray Burst VHE emission with the Southern Wide-field-of-view Gamma-ray Observatory, G. La Mura, U. Barres de Almeida, A. De Angelis, R. Conceição, F. Longo, M. Pimenta, E. Prandini, E. Ruiz-Velasco, B. Tomé on behalf of the SWGO Collaboration, 37th International Cosmic Ray Conference (Berlin)
41. The BepiColombo Radiation Monitor, Pinto, M., Gonçalves, P., Cardoso, C., Sanchez-Cano, B., Moissl, R., Vainio, R., Oleynik, P., Huovelin, J., Korpela, S., Lehtolainen, A., Grande, M., and Marques, A., Europlanet Science Congress 2021, <https://doi.org/10.5194/epsc2021-204>
42. Palestra/Webinar “Plantas ameaçadas de extinção - A Lista Vermelha da Flora Vascular de Portugal Continental”, por André Carapeto (Sociedade Portuguesa de Botânica), a 20 de Janeiro de 2021, integrada nas comemorações do Dia do Município de Vila do Bispo, organizada pela Sociedade Portuguesa de Botânica em parceria com a Câmara Municipal de Vila do Bispo.
43. Palestra/Webinar “A flora ameaçada no Município de Leiria”, por André Carapeto (Sociedade Portuguesa de Botânica), a 25 de Fevereiro de 2021, organizada pela Sociedade Portuguesa de Botânica em parceria com a Câmara Municipal de Leiria e o Centro de Interpretação Ambiental de Leiria.

Dataset

1. MOUTINHO CABRAL, I., MADEIRA, C., GROSSO, A.R., COSTA, P.M. Comparative transcriptomics between two potential toxin-secreting marine annelids: *Glycera alba* and *Hediste diversicolor*. GenBank OL606744-OL606747 (embargo pending)
2. Crispim Romao, Miguel; Castro, Nuno F.; Pedro, Rute; Simulated pp collisions at 13 TeV with 2 leptons + 1 b jet final state and selected benchmark Beyond the Standard Model signals. DOI: 10.5281/zenodo.5126747.

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