

2021

Journal Paper with direct contribution

1. de Almeida, Duarte Sampaio Belchior. Urban Tourism Crowding Dynamics: Carrying Capacity and Digital Twinning. Diss. ISCTE-Instituto Universitario de Lisboa (Portugal), 2021. <https://www.proquest.com/openview/e302b10227ebcf57af55fb137348500c/1?pq-origsite=gscholar&cbl=2026366&diss=y>
2. Almeida, Beatriz C., et al. "Transcription factor allosteric regulation through substrate coordination to zinc." *NAR genomics and bioinformatics* 3.2 (2021): lqab033. <https://doi.org/10.1093/nargab/lqab033>
3. Silva, João Manuel, et al. "Burden of Liver Cirrhosis in Portugal between 2010 and 2017." *GE-Portuguese Journal of Gastroenterology* 28.3 (2021): 153-161. <https://doi.org/10.1159/000510729>
4. Cabrita, Alexandra, et al. "Multiple pathways to homothallism in closely related yeast lineages in the Basidiomycota." *Mbio* 12.1 (2021): e03130-20. <https://doi.org/10.1128/mBio.03130-20>
5. Fortunato, A. B., et al. "Sediment dynamics and morphological evolution in the Tagus Estuary inlet." *Marine Geology* 440 (2021): 106590. <https://doi.org/10.1016/j.margeo.2021.106590>
6. Figueiredo, Pedro R., Ricardo D. González, and Alexandra TP Carvalho. "Human Carboxylesterase 2 in Cocaine Metabolism." *Molecular Catalysis* 515 (2021): 111938. <https://doi.org/10.1016/j.mcat.2021.111938>
7. Figueiredo, Pedro R., et al. "Introduction of a Glycine Linker Connecting the Heavy and Light Chains in Synthetic Cardosin B-Derived Rennet Changes the Specificity of Subpocket S3'." *The Journal of Physical Chemistry B* 125.17 (2021): 4368-4374. <https://doi.org/10.1021/acs.jpcc.1c01826>
8. Pinto, R., Sobral, D., Grosso, A.R. (2021). Comprehensive Detection of Pseudogenes Transcribed by Readthrough. In: Polisenio, L. (eds) *Pseudogenes. Methods in Molecular Biology*, vol 2324. Humana, New York, NY. https://doi.org/10.1007/978-1-0716-1503-4_6
9. Crispim Romão, M., Castro, N.F., Milhano, J.G. et al. Use of a generalized energy Mover's distance in the search for rare phenomena at colliders. *Eur. Phys. J. C* 81, 192 (2021). <https://doi.org/10.1140/epjc/s10052-021-08891-6>
10. Another look at the three-gluon vertex in the minimal Landau gauge, Guilherme T.R. Catumba (Coimbra U. and Valencia U., IFIC), Orlando Oliveira (Coimbra U.), Paulo J. Silva

(Coimbra U.) <https://doi.org/10.22323/1.396.0467>

11. PTPARL-D: an annotated corpus of forty-four years of Portuguese parliamentary debates Paulo Almeida, Manuel Marques-Pita, and Joana Gonçalves-Sá *Corpora* 2021 16:3, 337-348 <https://www.eupublishing.com/doi/full/10.3366/cor.2021.0226>
12. Borges, Sousa et al, 2021 (*Eurosurveillance*); <https://www.eurosurveillance.org/content/10.2807/1560-7917.ES.2021.26.10.2100130>
13. Borges, Isidro et al, 2021 (*Viruses*); <https://www.mdpi.com/1999-4915/13/4/604>
14. Borges, Isidro, Trovão et al, 2021 (pre-print in medRxiv); <https://www.medrxiv.org/content/10.1101/2021.02.22.21252216v1>
15. Borges et al, 2021 (pre-print in *Virological.org*); <https://virological.org/t/long-term-evolution-of-sars-cov-2-in-an-immunocompromised-patient-with-non-hodgkin-lymphoma/621>
16. Bento, et al. "Automated Analysis of Distributed Tracing: Challenges and Research Directions." *Journal of Grid Computing* 19.1 (2021): 1-15.
17. RODRIGO, A.P., GROSSO, A.R., BAPTISTA, P.V., FERNANDES, A.R., & COSTA, P.M. (2021). A transcriptomic approach to the recruitment of venom proteins in a marine annelid. *Toxins* 13, 97 (doi: 10.3390/toxins13020097).
18. RODRIGO, A.P., MENDES, V.M., MANADAS, B., GROSSO, A.R., ALVES DE MATOS, A.P., BAPTISTA, P.V., COSTA, P.M., FERNANDES, A.R. (2021). Specific antiproliferative properties of proteinaceous toxin secretions from the marine annelid *Eulalia* sp. onto ovarian cancer cells. *Marine Drugs* 19, 31 (doi: 10.3390/md19010031).
19. S. Aune, J. Bortfeldt, F. Brunbauer, C. David, D. Desforge, G. Fanourakis, M. Gallinaro, F. García, I. Giomataris, T. Gustavsson, F.J. Iguaz, M. Kebbiri, K. Kordas, C. Lampoudis, P. Legou, M. Lisowska, J. Liu, M. Lupberger, O. Maillard, I. Maniatis, I. Manthos, H. Müller, E. Oliveri, T. Papaevangelou, K. Paraschou, M. Pomorski, B. Qi, F. Resnati, L. Ropelewski, D. Sampsonidis, L. Scharenberg, T. Schneider, L. Sohl, M. van Stenis, A. Tsiamis, Y. Tsipolitis, S.E. Tzamarias, A. Utrobicic, R. Veenhof, X. Wang, S. White, Z. Zhang, Y. Zhou, Timing performance of a multi-pad PICOSEC-Micromegas detector prototype, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, Volume 993, 2021, <https://doi.org/10.1016/j.nima.2021.165076>
20. Rodrigues M, Martins R, Rogeiro J, Fortunato AB, Oliveira A, Cravo A, Jacob J, Rosa A, Azevedo A, Freire P. 2021 (in press). A web-based observatory for biogeochemical assessment in coastal regions, *Journal of Environmental Informatics*.
21. Rodrigues, M., A. Rosa, A. Cravo, Jacob, J., Fortunato, A.B. 2021 (in press). Effects of Climate Change and anthropogenic pressures in the water quality of a coastal lagoon (Ria Formosa, Portugal), *Science of the Total Environment*.
22. Rato, A.S., Alexandre, C.M., Almeida, P.R., Costa, J.L., Quintella, B.R. 2021. Effects of hydropeaking on the behaviour, fine-scale movements and habitat selection of an Iberian cyprinid fish. *River Research and Applications*
23. Sroczyńska, K., A. Conde, P. Chainho & H. Adão (2021). How nematode morphometric attributes integrate with taxonomy-based measures along an estuarine gradient. *Ecological Indicators* 124: 107384. <https://doi.org/10.1016/j.ecolind.2021.107384>
24. Mamede R, Vila-Cerqueira P, Silva M, Carriço JA, Ramirez M. 2021. Chewie Nomenclature Server (chewie-NS): a deployable nomenclature server for easy sharing of core and whole genome MLST schemas. *Nucleic Acids Res* 49:D660–D666. (PMID: 33068420)

25. MODELING THE IMPACTS OF HARBOR DREDGING AND DISPOSAL ON COASTAL WATER-LEVELS AND RUN-UP WITH XBEACH, Coastal Dynamics Conference, 28 June-2 July 2021.
26. Pereira, C., Maranha, J. R. e Cardoso R. (2021). A general mathematical framework for modelling soil-water retention behaviour. 3rd Pan-American Conference on Unsaturated Soils, Rio de Janeiro, Brazil (aceite para publicação).
27. CRAVO A., ROSA A., RODRIGUES M. (2020). Effects of climate change and anthropogenic pressures in the water quality of the Ria Formosa (Portugal). XX Seminário Ibérico de Química Marina - SIQUIMAR 2020, 1 pp.
28. Mendes, Lourenço S.; Lara, Javier L.; Viseu, Maria T. 2021. "Is the Volume-of-Fluid Method Coupled with a Sub-Grid Bubble Equation Efficient for Simulating Local and Continuum Aeration?" *Water* 13, no. 11: 1535.
29. Balduino César Mateus, Mateus Mendes, José Torres Farinha and António Marques Cardoso "Anticipating Future Behavior of an Industrial Press Using LSTM Networks" *Appl. Sci.* 2021, 11(13), 6101; <https://doi.org/10.3390/app11136101>
30. Paolillo, A., Sinval, J., Silva, S. A., & Scuderi, V. E. (2021). The relationship between inclusion climate and voice behaviors beyond social exchange obligation: The role of psychological needs satisfaction. *Sustainability*, 13(18), 1-19. <https://doi.org/10.3390/su131810252>
31. Balduino Mateus, Mateus Mendes, José Torres Farinha, António Marques Cardoso, *Data Analysis for Predictive Maintenance Using Time Series and Deep Learning Models - A Case Study in a Pulp Paper Industry*, in Proceedings of the TEPEN 2021 & IncoME-VI, Oct 20-23, 2021, Tianjin, China.
32. João Rodrigues, José Torres Farinha, António Marques Cardoso¹ and Mateus Mendes, *Prediction of Sensor Values in Paper Pulp Industry Using Neural Networks*, Proceedings of the TEPEN 2021 & IncoME-VI, Oct 20-23, 2021, Tianjin, China.
33. Pais, P., Oliveira, J., Almeida, V., Yilmaz, M., Monteiro, P.T., Teixeira, M.C. "Transcriptome-wide differences between *Saccharomyces cerevisiae* and *Saccharomyces cerevisiae* var. *boulardii*: clues on host survival and probiotic activity based on promoter sequence variability". *Genomics*, 113(2): 530-539, 2021.
34. Mendes S, et al. (2021) Genomic data and multi-species demographic modelling uncover past hybridization between currently allopatric freshwater species. *HEREDITY* <https://doi.org/10.1038/s41437-021-00466-1>.
35. Clemente F, et al. (2021) The genomic history of the Aegean palatial civilizations *CELL* 184: P2565-2586.e21 <https://doi.org/10.1016/j.cell.2021.03.039>
36. Palma JHN, 2017, CliPick - Climate change web picker. A tool bridging daily climate needs in process based modelling in forestry and agriculture, *Forest Systems [S.I.]*, v. 26, n. 1, p. eRC01, may 2017. ISSN 2171-9845. <https://doi.org/10.5424/fs/2017261-10251>
37. SANTOS, M.L., D'AMBROSIO, M., RODRIGO, A.P., PAROLA, A.J. & COSTA, P.M. (2021). A transcriptomic approach to the metabolism of tetrapyrrolic photosensitizers in a marine annelid. *Molecules* 26, 3924. (doi: 10.3390/molecules26133924).
38. RODRIGO, A.P., GROSSO, A.R., BAPTISTA, P.V., FERNANDES, A.R., & COSTA, P.M. (2021). A transcriptomic approach to the recruitment of venom proteins in a marine annelid. *Toxins* 13, 97 (doi: 10.3390/toxins13020097).
39. RODRIGO, A.P., MENDES, V.M., MANADAS, B., GROSSO, A.R., ALVES DE MATOS, A.P., BAPTISTA, P.V., COSTA, P.M., FERNANDES, A.R. (2021). Specific antiproliferative properties

- of proteinaceous toxin secretions from the marine annelid *Eulalia* sp. onto ovarian cancer cells. *Marine Drugs* 19, 31 (doi: 10.3390/md19010031).
40. Assessing the effects of PMM2 variants on protein stability Quelhas, D., Carneiro, J., Lopes-Marques, M., Jaeken, J., Martins, E., Rocha, J.F., Teixeira Carla, S.S., Ferreira, C.R., Sousa, S.F., Azevedo, L. (2021) *Molecular Genetics and Metabolism*, 134 (4), pp. 344-352. DOI: 10.1016/j.ymgme.2021.11.002
 41. In silico identification of possible inhibitors for protein kinase B (PknB) of mycobacterium tuberculosis Vieira, T.F., Martins, F.G., Moreira, J.P., Barbosa, T., Sousa, S.F. (2021) *Molecules*, 26 (20), art. no. 6162, .
 42. Structure and thermodynamics of empty clathrate hydrates below the freezing point of water† Fernando J. A. L. Cruz *a and José P. B. Motaa *Phys. Chem. Chem. Phys.*, 2021,23, 16033-16043 <https://doi.org/10.1039/D1CP00893E>
 43. The milk-derived lactoferrin inhibits V-ATPase activity by targeting its V1 domain Santos-Pereira, C., Rocha, J.F., Fernandes, H.S., Rodrigues, L.R., Côrte-Real, M., Sousa, S.F. (2021) *International Journal of Biological Macromolecules*, 186, pp. 54-70. DOI: 10.1016/j.ijbiomac.2021.06.200
 44. Compensatory epistasis explored by molecular dynamics simulations Serrano, C., Teixeira, C.S.S., Cooper, D.N., Carneiro, J., Lopes-Marques, M., Stenson, P.D., Amorim, A., Prata, M.J., Sousa, S.F., Azevedo, L. (2021) *Human Genetics*, 140 (9), pp. 1329-1342. DOI: 10.1007/s00439-021-02307-x
 45. The complete catalytic mechanism of xanthine oxidase: A computational study Ribeiro, P.M.G., Fernandes, H.S., Maia, L.B., Sousa, S.F., Moura, J.J.G., Cerqueira, N.M.F.S.A. (2021) *Inorganic Chemistry Frontiers*, 8 (2), pp. 405-416. DOI: 10.1039/d0qi01029d
 46. The Catalytic Mechanism of Pdx2 Glutaminase Driven by a Cys-His-Glu Triad: A Computational Study Pina, A.F., Sousa, S.F., Cerqueira, N.M.F.S.A. (2021) *ChemBioChem*, DOI: 10.1002/cbic.202100555
 47. New insights into the catalytic mechanism of the SARS-CoV-2 main protease: an ONIOM QM/MM approach Fernandes, H.S., Sousa, S.F., Cerqueira, N.M.F.S.A. (2021) *Molecular Diversity* DOI: 10.1007/s11030-021-10259-7
 48. Identification of new potential inhibitors of quorum sensing through a specialized multi-level computational approach Martins, F.G., Melo, A., Sousa, S.F. (2021) *Molecules*, 26 (9), art. no. 2600 DOI: 10.3390/molecules26092600
 49. Morgado P., L. Cavique (2021), Seleção de atributos usando LAID e sua implementação em sistemas de computação de alto desempenho, *Revista de Ciências da Computação* n.16, pp. 93-112.
 50. Finding new physics without learning about it: anomaly detection as a tool for searches at colliders M. Crispim Romao, N. F. Castro, R. Pedro *EPJC* 81 (2021) 27 *Jrn-Dir* 2021-01-15 10.1140/epjc/s10052-020-08807-w
 51. Light Higgs searches in $t\bar{t}$ production at the LHC Duarte Azevedo, Rodrigo Capucha, Emanuel Gouveia, Antonio Onofre, Rui Santos *J. High Energy Phys.* 4 (2021) 77 *Jrn-Dir* 2021-04-09 10.1007/JHEP04(2021)077
 52. Measurement of the associated production of a Higgs boson decaying into b-quarks with a vector boson at high transverse momentum in pp collisions at $\sqrt{s}=13\text{TeV}$ with the ATLAS detector ATLAS Collaboration (2927 authors) *Phys. Lett. B* 816 (2021) 136204 *Jrn-Dir* 2021-04-27 10.1016/j.physletb.2021.136204

53. A continuous integration and web framework in support of the ATLAS Publication Process
Juan Pedro Araque Espinosa, Gabriel Baldi Levcovitz, Riccardo-Maria Bianchi, Ian Brock,
Tancredi Carli, Nuno Filipe Castro, Alessandra Ciocio, Maurizio Colautti, Ana Carolina Da
Silva Menezes, Gabriel De Oliveira da Fonseca, Leandro Domingues Macedo Alves,
Andreas Hoecker, Bruno Lange Ramos, Gabriela Lemos Lúcidu Pinhão, Carmen
Maidantchik, Fairouz Malek, Robert McPherson, Gianluca Picco, Marcelo Teixeira Dos
Santos JINST 16 (2021) T05006 Jrn-Dir 2021-05-11 10.1088/1748-0221/16/05/T05006
54. Configuration and performance of the ATLAS b-jet triggers in Run 2 ATLAS Collaboration
Eur. Phys. J. C 81 (2021) 1087 Jrn-Dir 2021-12-01 10.1140/epjc/s10052-021-09775-5
55. Constraining the energy spectrum of neutral pions in ultra-high-energy proton-air
interactions Lorenzo Cazon, Ruben Conceição, Miguel Alexandre Martins, and Felix Riehn
Phys. Rev. D 103, 022001 Jrn-Dir 2021-01-08 10.1103/PhysRevD.103.022001
56. Measurement of the Fluctuations in the Number of Muons in Extensive Air Showers with
the Pierre Auger Observatory Pierre Auger Collaboration (360 authors) Phys. Rev. Lett.
126 (2021) 152002 Jrn-Dir 2021-04-16 10.1103/PhysRevLett.126.152002
57. Timing performance of a multi-pad PICOSEC-Micromegas detector prototype M. Gallinaro
et al. Nucl. Instrum. Methods Phys. Res. Sect. A-Accel. Spectrom. Dect. Assoc. Equip. 993
(2021) 165076 Jrn-Dir 2021-03-21 10.1016/j.nima.2021.165076
58. Modeling the timing characteristics of the PICOSEC Micromegas detector J. Bortfeldt et al.
(41 authors) Nucl. Instrum. Methods Phys. Res. Sect. A-Accel. Spectrom. Dect. Assoc.
Equip. 993 (2021) 165049 Jrn-Dir 2021-03-21 10.1016/j.nima.2021.165049
59. Measurement of the CP-violating phase $\phi(s)$ in the $B_s(0) \rightarrow J/\psi \phi(1020) \rightarrow \mu^+ \mu^- K^+ K^-$
channel in proton-proton collisions at $\sqrt{s}=13$ TeV CMS Collaboration (2307
authors) Phys. Lett. B 816 (2021) 136188 Jrn-Dir 2021-05-10
10.1016/j.physletb.2021.136188
60. Vector Boson Scattering Processes: Status and Prospects M. Gallinaro et al.
arXiv:2106.01393 Jrn-Dir 2021-06-02
61. Test beam characterization of sensor prototypes for the CMS Barrel MIP Timing Detector
CMS MTD Collaboration (199 authors) J. Instrum. 16 (2021) P07023 Jrn-Dir 2021-07-01
10.1088/1748-0221/16/07/P07023
62. Test beam characterization of sensor prototypes for the CMS Barrel MIP Timing Detector
D. Bastos, M. Gallinaro, T. Niknejad, J.C. Silva, J. Varela, et al. JINST 16 (2021) P07023 Jrn-
Dir 2021-07-15
63. Observation of B_0 s mesons and measurement of the B_0 s/ B^+ yield ratio in PbPb collisions
at 5.02 TeV CMS Collaboration arXiv:2109.01908 Jrn-Dir 2021-09-04
64. Advances in Multi-Variate Analysis Methods for New Physics Searches at the Large Hadron
Collider M. Gallinaro, G. Strong, J. Varela, et al. Rev.Phys. 7 (2021) 100063 Jrn-Dir 2021-
11-06
65. Improving sensitivity to low-mass dark matter in LUX using a novel electrode background
mitigation technique D. S. Akerib et al. Phys. Rev. D 104, 012011 Jrn-Dir 2021-07-19
<https://doi.org/10.1103/PhysRevD.104.012011>
66. Projected sensitivity of the LUX-ZEPLIN experiment to the two neutrino and neutrinoless
double beta decays in Xe-134 D. S. Akerib et al. Phys. Rev. C 104 (2021) 065501 Jrn-Dir
2021-12-10 <https://doi.org/10.1103/PhysRevC.104.065501>

67. Simulation of ^{125}I Auger emission spectrum with new atomic parameters from MCDHF calculations J.M. Sampaio, J. Ekman, B.P.E. Tee, R. du Rietz, B.Q. Lee, M.S. Pires, P. Jönsson, T. Kibédi, M. Vos, A.E. Stuchbery, and J.P. Marques *J. Quant. Spectr. Rad. Tranf.* 227, 107964 (2022) Jrn-Dir 2021-10-12 10.1016/j.jqsrt.2021.107964
68. Optical readout studies of the Thick-COBRA gaseous detector F. Garcia, F.M. Brunbauer, M. Lisowskac, H. Müller, E. Oliveri, D. Pfeiffer, L. Ropelewski, J. Samarati, F. Sauli, L. Scharenber, A.L.M. Silva, M. van Stenis, R. Veenhof and J.F.C.A. Veloso *JINST* 16 (2021) T01001 Jrn-Dir 2021-01-07 10.1088/1748-0221/16/01/T01001
69. Operation of a novel large area, high gain, single stage gaseous electron multiplier F.D. Amaro, R. Roque, N.V. Duarte, A. Cortez, and J.A. Mir *Journal of Instrumentation* 16 (2021) P01033 Jrn-Dir 2021-01-27 10.1088/1748-0221/16/01/P01033
70. Forecasting contrasting coastal and estuarine hydrodynamics with OPENCoastS A. Oliveira, A.B. Fortunato, M. Rodrigues, A. Azevedo, J. Rogeiro, S. Bernardo, Laura Lavaud, Xavier Bertin, Alphonse Nahon, Gonçalo de Jesus, Miguel Rocha, P. Lopes Anabela Oliveira, André B. Fortunato, Marta Rodrigues, Alberto Azevedo, João Rogeiro, Samuel Bernardo, Laura Lavaud, Xavier Bertin, Alphonse Nahon, Gonçalo de Jesus, Miguel Rocha, Pedro Lopes, Forecasting contrasting coastal and estuarine hydrodynamics with OPENCoastS, *Environmental Modelling & Software*, Volume 143, 2021 Jrn-Dir 2021-06-13 10.1016/j.envsoft.2021.105132
71. New methods to reconstruct X_{max} and the energy of gamma-ray air showers with high accuracy in large wide-field observatories R. Conceição, L. Peres, M. Pimenta, B. Tomé *Eur. Phys. J. C* 81, 80 (2021) Jrn-Dir 2021-01-25 10.1140/epjc/s10052-021-08883-6
72. Muon identification in a compact single-layered water Cherenkov detector and gamma/hadron discrimination using Machine Learning techniques R. Conceição, B. S. González, A. Guillén, M. Pimenta and B. Tomé *Eur. Phys. J. C* 81, 542 (2021) Jrn-Dir 2021-05-13 10.1140/epjc/s10052-021-09312-4
73. The SNO+ Experiment M.R. Anderson et al. (SNO+ Collaboration) *JINST* 16 P08059 (2021) Jrn-Dir 2021-08-25 10.1088/1748-0221/16/08/P08059
74. Optical calibration of the SNO+ detector in the water phase with deployed sources M.R. Anderson et al. (SNO+ Collaboration) *JINST* 16 P10021 Jrn-Dir 2021-10-19 10.1088/1748-0221/16/10/P10021
75. Quark Mass Function from an OGE-type Interaction in Minkowski Space E. P. Biernat, F. Gross, M. T. Peña, A. Stadler, S. Leitão *Acta Phys. Polon. Supp.* 14 (2021) 9 Jrn-Dir 2021-01-01 10.5506/APhysPolBSupp.14.9
76. Fundamental Parameters Related to Selenium $K\alpha$ and $K\beta$ Emission X-Ray Spectra Mauro Guerra, Jorge M. Sampaio, Gonçalo R. Vília, César A. Godinho, Daniel Pinheiro, Pedro Amaro, José P. Marques, Jorge Machado, Paul Indelicato, Fernando Parente, José Paulo Santos *Atoms* 9,8 (2021) Jrn-Dir 2021-01-22 10.3390/atoms 9010008
77. Peeling graphite layer by layer reveals the charge exchange dynamics of ions inside a solid Anna Niggas, Sascha Creutzburg, Janine Schwestka, Benjamin Wöckinger, Pedro L. Grande, Bernhard C. Bayer, José P. Marques, Friedrich Aumayr, Robert Bennett, Richard A. Wilhelm *Communications Physics* 4, 1801 (2021). Jrn-Dir 2021-08-12 10.1038/s42005-021-00686-1
78. NeuLAND: The high-resolution neutron time-of-flight spectrometer for R3B at FAIR K. Boretzky, I. Gasparic, M. Heil, et al. *Nucl. Instr. and Methods A* 1014, 165071 (2021) Jrn-Dir

2021-10-21 10.1016/j.nima.2021.165701

79. The large COMPASS polarized solid ammonia target for Drell-Yan measurements with a pion beam V. Andrieux, C. Pires, C. Quintans et al NIM A 1025 (2022) 166069 Jrn-Dir 2021-12-10 <https://doi.org/10.1016/j.nima.2021.166069>
80. Constraining the energy spectrum of neutral pions in ultra-high-energy proton-air interactions Lorenzo Cazon, Ruben Conceição, Miguel Alexandre Martins, and Felix Riehn Phys. Rev. D 103, 022001 Jrn-Dir 2021-01-08 10.1103/PhysRevD.103.022001
81. Running in the ALPs M. Chala, G. Guedes, M. Ramos and J. Santiago Eur. Phys. J. C (2021) 81: 181 Jrn-Dir 2021-02-23 10.1140/epjc/s10052-021-08968-2
82. Use of a Generalized Energy Mover's Distance in the Search for Rare Phenomena at Colliders M. Crispim Romao, N.F. Castro , J.G. Milhano, R. Pedro, T. Vale Eur. Phys. J. C 81, 192 (2021) Jrn-Dir 2021-02-26 10.1140/epjc/s10052-021-08891-6
83. New leptons with exotic decays: collider limits and dark matter complementarity Guilherme Guedes, José Santiago arXiv:2107.03429 Jrn-Dir 2021-07-09
84. Deep Learning for the Classification of Quenched Jets L. Apolinário, N. F. Castro, M. Crispim Romão, J. G. Milhano, R. Pedro, F. C. R. Peres JHEP11 (2021) 219 Jrn-Dir 2021-11-29 10.1007/JHEP11(2021)219
85. Finding new physics without learning about it: anomaly detection as a tool for searches at colliders M. Crispim Romao, N. F. Castro, R. Pedro EPJC 81 (2021) 27 Jrn-Dir 2021-01-15 10.1140/epjc/s10052-020-08807-w
86. Use of a Generalized Energy Mover's Distance in the Search for Rare Phenomena at Colliders M. Crispim Romao, N.F. Castro , J.G. Milhano, R. Pedro, T. Vale Eur. Phys. J. C 81, 192 (2021) Jrn-Dir 2021-02-26 10.1140/epjc/s10052-021-08891-6
87. A continuous integration and web framework in support of the ATLAS Publication Process Juan Pedro Araque Espinosa, Gabriel Baldi Levcovitz, Riccardo-Maria Bianchi, Ian Brock, Tancredi Carli, Nuno Filipe Castro, Alessandra Ciocio, Maurizio Colautti, Ana Carolina Da Silva Menezes, Gabriel De Oliveira da Fonseca, Leandro Domingues Macedo Alves, Andreas Hoecker, Bruno Lange Ramos, Gabriela Lemos Lúcidu Pinhão, Carmen Maidantchik, Fairouz Malek, Robert McPherson, Gianluca Picco, Marcelo Teixeira Dos Santos JINST 16 (2021) T05006 Jrn-Dir 2021-05-11 10.1088/1748-0221/16/05/T05006
88. Deep Learning for the Classification of Quenched Jets L. Apolinário, N. F. Castro, M. Crispim Romão, J. G. Milhano, R. Pedro, F. C. R. Peres JHEP11 (2021) 219 Jrn-Dir 2021-11-29 10.1007/JHEP11(2021)219
89. A source of very energetic oxygen located in Jupiter's inner radiation belts Elias Roussos, Christina Cohen, Peter Kollmann, Marco Pinto, Norbert Krupp, Patricia Gonçalves, Konstantinos Dialynas Space Advances, Vol 8, Issue 2 Jrn-Dir 2022-01-14 DOI: 10.1126/sciadv.abm4234
90. Fortunato, A.B., P. Freire, B. Mengual, X. Bertin, C. Pinto, K. Martins, T. Guérin, A. Azevedo 2021. Sediment dynamics and morphological evolution in the Tagus Estuary inlet, Marine Geology, 440: 106590. DOI: 10.1016/j.margeo.2021.106590
91. Oliveira, A., A.B. Fortunato, M. Rodrigues, A. Azevedo, J. Rogeiro, S. Bernardes, L. Lavaud, X. Bertin, A. Nahon, G. Jesus, M. Rocha, P. Lopes 2021. Forecasting contrasting coastal and estuarine hydrodynamics with OPENCoastS, Environmental Modelling & Software, 143: 105132. DOI: 10.1016/j.envsoft.2021.105132

92. Rocha, M; Oliveira, A.; Freire, P.; Fortunato, A.B.; Nahon, A.; Barros, J.L.; Azevedo, A.; Oliveira, F.S.B.F.; Rogeiro, J.; Jesus, G.; Martins, R.J.; Santos, P.P.; Tavares, A.O.; Oliveira, J. 2021. Multi-Hazard WebGIS Platform for Coastal Regions, APPLIED SCIENCES-BASEL, 11/11: 5253, DOI: 10.3390/app11115253
93. Rodrigues, M., R. Martins, J. Rogeiro, A. B. Fortunato, A. Oliveira, A. Cravo, J. Jacob, A. Rosa, A. Azevedo, P. Freire 2021. A Web-Based Observatory for Biogeochemical Assessment in Coastal Regions, Journal of Environmental Informatics, 38/1: 1.15. DOI:10.3808/jei.202100450
94. Fassoni-Andrade, A. C., Durand, F., Moreira, D., Azevedo, A., dos Santos, V. F., Funi, C., and Laraque, A.: Comprehensive bathymetry and intertidal topography of the Amazon estuary, Earth Syst. Sci. Data, 13, 2275–2291, <https://doi.org/10.5194/essd-13-2275-2021>, 2021.

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
3. 2020.09087.BD
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

- Tecnologia da Universidade Nova de Lisboa, Monte de Caparica. 43 pp. + Appendix. Final status: Approved. Classification: 18 (0-20).
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 Vasculare 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 GASPAS 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 Vasculare 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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