# FULL LIST OF PUBLICATIONS

*Sérgio F. Sousa (BIA Lab / BioSIM)*

## 2026

168. Selvam R., Yap M.K.K., Giacomazzi R., Sousa S.F., Tan H.S. **Aptamer-mediated outer membrane destabilization overcomes low permeability resistance in Pseudomonas aeruginosa**. *The FEBS Journal* **(2026)**. doi: 10.1111/febs.70560. 0 citations

167. Martins F.G., Santos H.A., Sousa S.F. **A Review of Current Computational Tools for Peptide–Protein Docking**. *Journal of Computational Chemistry* **(2026)**. doi: 10.1002/jcc.70328. 1 citations

166. Salgado Pires V., Pires Gravina-Oliveira M., Silva-Junior N., Saraiva Veloso B., Maia de Sousa S.F., Dias Mesquita R. **Structural comparison between human and Leishmania infantum Sirtuin 2 NAD-dependent histone deacetylases**. *Acta Tropica* **(2026)**. doi: 10.1016/j.actatropica.2026.107969. 0 citations

165. Salman M.K., Giordano I., Tommonaro G., Cutignano A., Sousa S.F., Borges A., Mauriello G., Abbamondi G.R. **Characterization of AHL-mediated quorum sensing in Pseudomonas gessardii from raw milk and insights into control of proteolytic activity**. *International Journal of Food Microbiology* **(2026)**. doi: 10.1016/j.ijfoodmicro.2025.111502. 1 citations

164. Lopez-Parra J.S., Hameedat F., Sousa S.F., Walenkamp A.M.E., Sousa F., A Santos H. **Identification of Subtype-Specific Vulnerabilities in Resistant Glioblastoma: A Computational Pipeline for Biomarkers and Drug Discovery**. *Molecular Pharmaceutics* **(2026)**. doi: 10.1021/acs.molpharmaceut.5c01538. 0 citations

## 2025

163. Singh M., Karthikeyan C., Waiker D.K., Tiwari A., Shrivastava S.K., Sousa S.F., Kiriwan D., Martins F.G., Moorthy N.S.H.N. **Design, synthesis, and pharmacological evaluation of heteroaryl thiol-linked kojic acid derivatives as a novel class of acetylcholinesterase inhibitors for Alzheimer's disease therapy**. *3 Biotech* **(2025)**. doi: 10.1007/s13205-025-04295-5. 4 citations

162. Roggero A., Toyama M.H., Sousa S.F. **Lands' Cycle at the Crossroads: Phospholipid Remodelling, Oxidative Stress, Cellular Toxicity, and Therapeutic Targeting**. *ACS Pharmacology and Translational Science* **(2025)**. doi: 10.1021/acsptsci.5c00482. 2 citations

161. Leitão M.M., Gonçalves A.S.C., Sousa S.F., Borges F., Simões M., Borges A. **Two cinnamic acid derivatives as inhibitors of Pseudomonas aeruginosa las and pqs quorum-sensing systems: Impact on biofilm formation and virulence factors**. *Biomedicine and Pharmacotherapy* **(2025)**. doi: 10.1016/j.biopha.2025.118090. 10 citations

160. Roggero A., Loyola P.M., Ramos da Cruz C., Santos W.H.B.C., Borges P.P., dos Santos Junior A.B., Martins F., Oliveira M.A., Sousa S.F., Toyama M.H. **NSAIDs beyond COX: In Silico and In Vitro Insights into Acetylcholinesterase Modulation**. *ACS Omega* **(2025)**. doi: 10.1021/acsomega.5c08750. 0 citations

159. Filho J.L.P., Pereira R.B., Vieira T.F., Sousa S.F., Coelho J.R.A., Pinto N.F.S., Coelho C.M.M., Fernandes M.J.G., Castanheira E.M.S., Gonçalves M.S.T., Pereira D.M. **Development of eugenol derivatives with 5-LOX inhibitory activity**. *Journal of Enzyme Inhibition and Medicinal Chemistry* **(2025)**. doi: 10.1080/14756366.2025.2535586. 0 citations

158. Kiriwan D., Vieira T.F., Kumsiri N., Sousa S.F., Choowongkomon K. **Identification of Tripeptide Inhibitors Targeting MAPK3 in Leishmania martiniquensis and Leishmania orientalis Using Molecular Modeling, Virtual Screening, Molecular Dynamics, and In Vitro Approach**. *ACS Omega* **(2025)**. doi: 10.1021/acsomega.5c03481. 0 citations

157. Peixoto V.P., Prudêncio C., Vieira M., Sousa S.F. **Evaluation of the impact of two C5 genetic variants on C5-eculizumab complex stability at the molecular level**. *Journal of Biomolecular Structure and Dynamics* **(2025)**. doi: 10.1080/07391102.2024.2331091. 0 citations

156. Oliveira T., Ferraz R., Azevedo L., Quelhas D., Carneiro J., Jaeken J., Sousa S.F. **A comprehensive update of genotype–phenotype correlations in PMM2-CDG: insights from molecular and structural analyses**. *Orphanet Journal of Rare Diseases* **(2025)**. doi: 10.1186/s13023-025-03669-5. 4 citations

155. Singh S., Paul S., Martins F.G., Sousa S.F., Kundu C.N., Karthikeyan C., Moorthy N.S.H.N. **Design, synthesis and biological evaluation of 2-phenylquinoxaline carbonyl piperazine derivatives as novel FASN inhibitors with anticancer activity**. *Bioorganic Chemistry* **(2025)**. doi: 10.1016/j.bioorg.2025.108697. 1 citations

## 2024

154. Thakur C.K., Martins F.G., Karthikeyan C., Bhal S., Kundu C.N., Moorthy N.S.H.N., Sousa S.F. **In silico-guided discovery and in vitro validation of novel sugar-tethered lysinated carbon nanotubes for targeted drug delivery of doxorubicin**. *Journal of Molecular Modeling* **(2024)**. doi: 10.1007/s00894-024-06061-5. 3 citations

153. Leitão M.M., Vieira T.F., Sousa S.F., Borges F., Simões M., Borges A. **Dual action of benzaldehydes: Inhibiting quorum sensing and enhancing antibiotic efficacy for controlling Pseudomonas aeruginosa biofilms**. *Microbial Pathogenesis* **(2024)**. doi: 10.1016/j.micpath.2024.106663. 16 citations

152. Vieira T.F., Leitão M.M., Cerqueira N.M.F.S.A., Sousa S.F., Borges A., Simões M. **Montelukast and cefoperazone act as antiquorum sensing and antibiofilm agents against Pseudomonas aeruginosa**. *Journal of Applied Microbiology* **(2024)**. doi: 10.1093/jambio/lxae088. 6 citations

151. Fernandes S., Sousa M., Martins F.G., Simões M., Sousa S.F. **Protocol for in silico characterization of natural-based molecules as quorum-sensing inhibitors**. *STAR Protocols* **(2024)**. doi: 10.1016/j.xpro.2024.103367. 2 citations

150. Zeghbib W., Boudjouan F., Carneiro J., Oliveira A.L.S., Sousa S.F., Pintado M.E., Ourabah A., Vasconcelos V., Lopes G. **LC-ESI-UHR-QqTOF-MS/MS profiling and anti-inflammatory potential of the cultivated Opuntia ficus-indica (L.) Mill. and the wild Opuntia stricta (Haw.) Haw. fruits from the Algerian region**. *Food Chemistry* **(2024)**. doi: 10.1016/j.foodchem.2024.140414. 13 citations

149. Araškov J.B., Garcia-Sosa A.T., Višnjevac A., Sousa S.F., Holló B.B., Uğuz Ö., Koca A., Monge M., Rodríguez-Castillo M., López-de-Luzuriaga J.M., Todorović T.R., Filipović N.R. **Structural insights and photophysical properties of mononuclear and pentanuclear Zn(II) acetate complexes with pyridyl-based thiazolyl-hydrazones**. *Polyhedron* **(2024)**. doi: 10.1016/j.poly.2024.117162. 3 citations

148. Mendes F., Santos-Pereira C., Vieira T.F., Martins Pinto M., Castro B.B., Sousa S.F., Sousa M.J., Devin A., Chaves S.R. **The fungicide cymoxanil impairs respiration in Saccharomyces cerevisiae via cytochrome c oxidase inhibition**. *FEBS Letters* **(2024)**. doi: 10.1002/1873-3468.14907. 2 citations

147. Duarte-Silva S., Da Silva J.D., Monteiro-Fernandes D., Costa M.D., Neves-Carvalho A., Raposo M., Soares-Cunha C., Correia J.S., Nogueira-Goncalves G., Fernandes H.S., Oliveira S., Ferreira-Fernandes A.R., Rodrigues F., Pereira-Sousa J., Vilasboas-Campos D., Guerreiro S., Campos J., Meireles-Costa L., Rodrigues C.M.P., Cabantous S., Sousa S.F., Lima M., Teixeira-Castro A., Maciel P. **Glucocorticoid receptor-dependent therapeutic efficacy of tauroursodeoxycholic acid in preclinical models of spinocerebellar ataxia type 3**. *Journal of Clinical Investigation* **(2024)**. doi: 10.1172/JCI162246. 12 citations

146. Soares R., Azevedo L., Vasconcelos V., Pratas D., Sousa S.F., Carneiro J. **Machine Learning-Driven Discovery and Database of Cyanobacteria Bioactive Compounds: A Resource for Therapeutics and Bioremediation**. *Journal of Chemical Information and Modeling* **(2024)**. doi: 10.1021/acs.jcim.4c00995. 4 citations

145. Paquete-Ferreira J., Freire F., Fernandes H.S., Muthukumaran J., Ramos J., Bryton J., Panjkovich A., Svergun D., Santos M.F.A., Correia M.A.S., Fernandes A.R., Romão M.J., Sousa S.F., Santos-Silva T. **Structural insights of an LCP protein–LytR–from Streptococcus dysgalactiae subs. dysgalactiae through biophysical and in silico methods**. *Frontiers in Chemistry* **(2024)**. doi: 10.3389/fchem.2024.1379914. 5 citations

144. Sousa J., Santos-Pereira C., Gomes J.S., Costa Â.M.A., Santos A.O., Franco-Duarte R., Linhares J.M.M., Sousa S.F., Silvério S.C., Rodrigues L.R. **Heterologous expression and structure prediction of a xylanase identified from a compost metagenomic library**. *Applied Microbiology and Biotechnology* **(2024)**. doi: 10.1007/s00253-024-13169-4. 7 citations

143. Batista-Silva J.P., Gomes D., Sousa S.F., Sousa Â., Passarinha L.A. **Advances in structure-based drug design targeting membrane protein markers in prostate cancer**. *Drug Discovery Today* **(2024)**. doi: 10.1016/j.drudis.2024.104130. 5 citations

142. Vasconcelos D., Pina A., Habib N., Sousa S. **In silico analysis of aptamer-RNA conjugate interactions with human transferrin receptor**. *Biophysical Chemistry* **(2024)**. doi: 10.1016/j.bpc.2024.107308. 5 citations

141. Ferreiro D., Khalil R., Sousa S.F., Arenas M. **Substitution Models of Protein Evolution with Selection on Enzymatic Activity**. *Molecular Biology and Evolution* **(2024)**. doi: 10.1093/molbev/msae026. 3 citations

## 2023

140. Carneiro J., Magalhães R.P., de la Oliva Roque V.M., Simões M., Pratas D., Sousa S.F. **TargIDe: a machine-learning workflow for target identification of molecules with antibiofilm activity against Pseudomonas aeruginosa**. *Journal of Computer-Aided Molecular Design* **(2023)**. doi: 10.1007/s10822-023-00505-5. 9 citations

139. Teixeira C.S.S., Biltes R., Villa C., Sousa S.F., Costa J., Ferreira I.M.P.L.V.O., Mafra I. **Exploiting Locusta migratoria as a source of bioactive peptides with anti-fibrosis properties using an in silico approach**. *Food and Function* **(2023)**. doi: 10.1039/d3fo04246d. 5 citations

138. Teixeira C.S.S., Villa C., Sousa S.F., Costa J., Ferreira I.M.P.L.V.O., Mafra I. **An in silico approach to unveil peptides from Acheta domesticus with potential bioactivity against hypertension, diabetes, cardiac and pulmonary fibrosis**. *Food Research International* **(2023)**. doi: 10.1016/j.foodres.2023.112847. 16 citations

137. Araškov J.B., Maciejewska N., Olszewski M., Višnjevac A., Blagojević V., Fernandes H.S., Sousa S.F., Puerta A., Padrón J.M., Holló B.B., Monge M., Rodríguez-Castillo M., López-de-Luzuriaga J.M., Uğuz Ö., Koca A., Todorović T.R., Filipović N.R. **Structural, physicochemical and anticancer study of Zn complexes with pyridyl-based thiazolyl-hydrazones**. *Journal of Molecular Structure* **(2023)**. doi: 10.1016/j.molstruc.2023.135157. 9 citations

136. Araújo M.F., Castanheira E.M.S., Sousa S.F. **The Buzz on Insecticides: A Review of Uses, Molecular Structures, Targets, Adverse Effects, and Alternatives**. *Molecules* **(2023)**. doi: 10.3390/molecules28083641. 143 citations

135. Vieira T.F., Cerqueira N.M.F.S.A., Simões M., Sousa S.F. **In silico identification of novel PqsD inhibitors: promising molecules for quorum sensing interference in Pseudomonas aeruginosa**. *Molecular Systems Design and Engineering* **(2023)**. doi: 10.1039/d3me00107e. 5 citations

134. Belchor M.N., Costa C.R.D.C., Roggero A., Moraes L.L.F., Samelo R., Annunciato I., de Oliveira M.A., Sousa S.F., Toyama M.H. **In Silico Evaluation of Quercetin Methylated Derivatives on the Interaction with Secretory Phospholipases A2 from Crotalus durissus terrificus and Bothrops jararacussu**. *Pharmaceuticals* **(2023)**. doi: 10.3390/ph16040597. 4 citations

133. Costa C.R.C., Belchor M.N., Roggero A., Moraes L.L., Samelo R., Annunciato I., Bonturi C.R., Oliva M.L.V., Sousa S.F., de Oliveira M.A., Toyama M.H. **The First Anti-Snakebite and Hepatoprotective Characterization of a Trypsin Kunitz-like Inhibitor (EcTI) from the Plant Enterolobium contortisiliquum; A Case of Two Soul Mates Meeting**. *Pharmaceuticals* **(2023)**. doi: 10.3390/ph16040632. 1 citations

132. Leite J.P., Lourenço F., Oliveira R., Sousa S.F., Mendes M.V., Gales L. **Crystal structures of Streptomyces tsukubaensis sigma factor SigG1 and anti-sigma RsfG**. *Journal of Structural Biology* **(2023)**. doi: 10.1016/j.jsb.2023.108038. 2 citations

131. Vieira T.F., Sousa S.F. **Receptor-Based Virtual Screening of Large Libraries in a Multi-Level In Silico Approach**. *Methods in Molecular Biology* **(2023)**. doi: 10.1007/978-1-0716-3147-8_15. 3 citations

130. Mauro E., Lapaillerie D., Tumiotto C., Charlier C., Martins F., Sousa S.F., Métifiot M., Weigel P., Yamatsugu K., Kanai M., Munier-Lehmann H., Richetta C., Maisch M., Dutrieux J., Batisse J., Ruff M., Delelis O., Lesbats P., Parissi V. **Modulation of the functional interfaces between retroviral intasomes and the human nucleosome**. *mBio* **(2023)**. doi: 10.1128/mbio.01083-23. 4 citations

129. Fernandes S., Borges A., Gomes I.B., Sousa S.F., Simões M. **Curcumin and 10-undecenoic acid as natural quorum sensing inhibitors of LuxS/AI-2 of Bacillus subtilis and LasI/LasR of Pseudomonas aeruginosa**. *Food Research International* **(2023)**. doi: 10.1016/j.foodres.2023.112519. 51 citations

128. Martins F.G., Thakur C.K., Karthikeyan C., Moorthy N.S.H.N., Sousa S.F. **Use of lysinated multiwalled carbon nanotubes with carbohydrate ligands as a doxorubicin nanocarrier: A molecular dynamics analysis**. *Carbon Trends* **(2023)**. doi: 10.1016/j.cartre.2023.100280. 6 citations

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125. Teixeira C.S.S., Sousa S.F. **Current status of the use of multifunctional enzymes as anti-cancer drug targets**. *Pharmaceutics* **(2022)**. doi: 10.3390/pharmaceutics14010010. 12 citations

124. Sousa S.F. **Special Issue on "Enzymes as Biocatalysts: Current Research Trends and Applications"**. *International Journal of Molecular Sciences* **(2022)**. doi: 10.3390/ijms232416209. 2 citations

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122. Marković S.B., Maciejewska N., Olszewski M., Višnjevac A., Puerta A., Padrón J.M., Novaković I., Kojić S., Fernandes H.S., Sousa S.F., Ramotowska S., Chylewska A., Makowski M., Todorović T.R., Filipović N.R. **Study of the anticancer potential of Cd complexes of selenazoyl-hydrazones and their sulfur isosters**. *European Journal of Medicinal Chemistry* **(2022)**. doi: 10.1016/j.ejmech.2022.114449. 22 citations

121. Silva S., Marto J., Gonçalves L.M., Fernandes H.S., Sousa S.F., Almeida A.J., Vale N. **Development of Neuropeptide Y and Cell-Penetrating Peptide MAP Adsorbed onto Lipid Nanoparticle Surface**. *Molecules* **(2022)**. doi: 10.3390/molecules27092734. 13 citations

120. Pina A.F., Sousa S.F., Cerqueira N.M.F.S.A. **The Catalytic Mechanism of Pdx2 Glutaminase Driven by a Cys-His-Glu Triad: A Computational Study**. *ChemBioChem* **(2022)**. doi: 10.1002/cbic.202100555. 3 citations

119. Magalhães R.P., Vieira T.F., Melo A., Sousa S.F. **Identification of novel candidates for inhibition of LasR, a quorum-sensing receptor of multidrug resistant Pseudomonas aeruginosa, through a specialized multi-level in silico approach**. *Molecular Systems Design and Engineering* **(2022)**. doi: 10.1039/d2me00009a. 21 citations

118. Lapaillerie D., Charlier C., Guyonnet-Dupérat V., Murigneux E., Fernandes H.S., Martins F.G., Magalhães R.P., Vieira T.F., Richetta C., Subra F., Lebourgeois S., Charpentier C., Descamps D., Visseaux B., Weigel P., Favereaux A., Beauvineau C., Buron F., Teulade-Fichou M.-P., Routier S., Gallois-Montbrun S., Meertens L., Delelis O., Sousa S.F., Parissi V. **Selection of Bis-Indolyl Pyridines and Triphenylamines as New Inhibitors of SARS-CoV-2 Cellular Entry by Modulating the Spike Protein/ACE2 Interfaces**. *Antimicrobial Agents and Chemotherapy* **(2022)**. doi: 10.1128/aac.00083-22. 16 citations

117. Fernandes S., Gomes I.B., Sousa S.F., Simões M. **Antimicrobial Susceptibility of Persister Biofilm Cells of Bacillus cereus and Pseudomonas fluorescens**. *Microorganisms* **(2022)**. doi: 10.3390/microorganisms10010160. 26 citations

116. Vieira T.F., Magalhães R.P., Cerqueira N.M.F.S.A., Simões M., Sousa S.F. **Targeting Pseudomonas aeruginosa MvfR in the battle against biofilm formation: a multi-level computational approach**. *Molecular Systems Design and Engineering* **(2022)**. doi: 10.1039/d2me00088a. 6 citations

115. Araškov J.B., Višnjevac A., Popović J., Blagojević V., Fernandes H.S., Sousa S.F., Novaković I., Padrón J.M., Holló B.B., Monge M., Rodríguez-Castillo M., López-De-Luzuriaga J.M., Filipović N.R., Todorović T.R. **Zn(ii) complexes with thiazolyl-hydrazones: structure, intermolecular interactions, photophysical properties, computational study and anticancer activity**. *CrystEngComm* **(2022)**. doi: 10.1039/d2ce00443g. 17 citations

114. Pina A.F., Sousa S.F., Azevedo L., Carneiro J. **Non-B DNA conformations analysis through molecular dynamics simulations**. *Biochimica et Biophysica Acta - General Subjects* **(2022)**. doi: 10.1016/j.bbagen.2022.130252. 7 citations

113. Vieira T.F., Magalhães R.P., Simões M., Sousa S.F. **Drug Repurposing Targeting Pseudomonas aeruginosa MvfR Using Docking, Virtual Screening, Molecular Dynamics, and Free-Energy Calculations**. *Antibiotics* **(2022)**. doi: 10.3390/antibiotics11020185. 36 citations

112. Pereira A.C., Pina A.F., Sousa D., Ferreira D., Santos-Pereira C., Rodrigues J.L., Melo L.D.R., Sales G., Sousa S.F., Rodrigues L.R. **Identification of novel aptamers targeting cathepsin B-overexpressing prostate cancer cells**. *Molecular Systems Design and Engineering* **(2022)**. doi: 10.1039/d2me00022a. 9 citations

111. Fernandes H.S., Sousa S.F., Cerqueira N.M.F.S.A. **New insights into the catalytic mechanism of the SARS-CoV-2 main protease: an ONIOM QM/MM approach**. *Molecular Diversity* **(2022)**. doi: 10.1007/s11030-021-10259-7. 30 citations

110. Burke A.J., Teixeira C.S.S., Sousa S.F. **Transformation of a Chiral Glycolic Acid to an Isoaurone: Stereochemical Assignment of a Benzilic Acid Rearrangment Product**. *Asian Journal of Organic Chemistry* **(2022)**. doi: 10.1002/ajoc.202100692. 0 citations

109. Fernandes H.S., Cerqueira N.M.F.S.A., Sousa S.F., Melo A. **A Molecular Mechanics Energy Partitioning Software for Biomolecular Systems**. *Molecules* **(2022)**. doi: 10.3390/molecules27175524. 2 citations

108. Rocha J.F., Sousa S.F., Cerqueira N.M.F.S.A. **Computational Studies Devoted to the Catalytic Mechanism of Threonine Aldolase, a Critical Enzyme in the Pharmaceutical Industry to Synthesize β-Hydroxy-α-amino Acids**. *ACS Catalysis* **(2022)**. doi: 10.1021/acscatal.1c05567. 15 citations

107. Kiriwan D., Seetaha S., Jiwacharoenchai N., Tabtimmai L., Sousa S.F., Songtawee N., Choowongkomon K. **Identification of tripeptides against tyrosine kinase domain of EGFR for lung cancer cell inhibition by in silico and in vitro studies**. *Chemical Biology and Drug Design* **(2022)**. doi: 10.1111/cbdd.14010. 9 citations

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106. Lapaillerie D., Charlier C., Fernandes H.S., Sousa S.F., Lesbats P., Weigel P., Favereaux A., Guyonnet-Duperat V., Parissi V. **In silico, in vitro and in cellulo models for monitoring sars-cov-2 spike/human ace2 complex, viral entry and cell fusion**. *Viruses* **(2021)**. doi: 10.3390/v13030365. 14 citations

105. Fernandes H.S., Cerqueira N.M.F.S.A., Sousa S.F. **Developing and Using BioSIMAR, an Augmented Reality Program to Visualize and Learn about Chemical Structures in a Virtual Environment on Any Internet-Connected Device**. *Journal of Chemical Education* **(2021)**. doi: 10.1021/acs.jchemed.0c01317. 18 citations

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103. 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. **Assessing the effects of PMM2 variants on protein stability**. *Molecular Genetics and Metabolism* **(2021)**. doi: 10.1016/j.ymgme.2021.11.002. 6 citations

102. Sousa S.F. **Special issue on "the application of quantum mechanics in reactivity of molecules"**. *Applied Sciences (Switzerland)* **(2021)**. doi: 10.3390/app11031132. 0 citations

101. Santos-Pereira C., Rocha J.F., Fernandes H.S., Rodrigues L.R., Côrte-Real M., Sousa S.F. **The milk-derived lactoferrin inhibits V-ATPase activity by targeting its V1 domain**. *International Journal of Biological Macromolecules* **(2021)**. doi: 10.1016/j.ijbiomac.2021.06.200. 12 citations

100. Silva Teixeira C.S., Sousa S.F., Cerqueira N.M.F.S.A. **An Unsual Cys-Glu-Lys Catalytic Triad is Responsible for the Catalytic Mechanism of the Nitrilase Superfamily: A QM/MM Study on Nit2**. *ChemPhysChem* **(2021)**. doi: 10.1002/cphc.202000751. 17 citations

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98. Mihaljević-Jurič P., Sousa S.F. **A QM/MM evaluation of the missing step in the reduction mechanism of HMG-CoA by human HMG-CoA reductase**. *Processes* **(2021)**. doi: 10.3390/pr9071085. 2 citations

97. Martins F.G., Melo A., Sousa S.F. **Databases for the study of biofilms: current status and potential applications**. *Biofouling* **(2021)**. doi: 10.1080/08927014.2021.1876849. 6 citations

96. Martins F.G., Melo A., Sousa S.F. **Identification of new potential inhibitors of quorum sensing through a specialized multi-level computational approach**. *Molecules* **(2021)**. doi: 10.3390/molecules26092600. 30 citations

95. Magalhães R.P., Cunha J.M., Sousa S.F. **Perspectives on the role of enzymatic biocatalysis for the degradation of plastic pet**. *International Journal of Molecular Sciences* **(2021)**. doi: 10.3390/ijms222011257. 81 citations

94. Vieira T.F., Martins F.G., Moreira J.P., Barbosa T., Sousa S.F. **In silico identification of possible inhibitors for protein kinase B (PknB) of mycobacterium tuberculosis**. *Molecules* **(2021)**. doi: 10.3390/molecules26206162. 13 citations

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