Matheus Ferraz

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Research Interest

My primary research interests consist of the application of computational chemistry methodologies to study condensed phase matter. My work portfolio consists of understanding the theoretical aspects of biological systems and designing novel proteins with engineered functions. I am particularly keen on developing and applying Machine/deep learning (ML/DL) methodologies to guide the design of nanobodies (Nbs) targeting several antigenic targets. It also includes the use of classical molecular dynamics simulations to assess the stability and conformational dynamism of the designed Nbs. Moreover, I have been applying ML/DL algorithms to offer an enhanced insight into protein biophysics.

Education

2019 – Present	Ph.D. Chemistry, Federal University of Pernambuco, Brazil Exchange Period at the Heidelberg Institute for Theoretical Studies (Under the supervision of Dr. Rebecca C. Wade, DAAD scholarship recipient starting October 2021) Thesis: Nanobodies Engineering Assisted by Machine Learning Methods Advisor: Dr. Roberto Lins
2013 – 2018	B. Eng. Chemical Engineering, Federal University of Pernambuco, Brazil Monography: Multiscale Simulations Tools: Development of ZIKV diagnostic raw material and industrial scale-up of its production Advisor: Dr. Sergio Lucena

Awards

- Highlighted talk by the Federal Chemistry Council from Brazil, 2021;
- Best posters presented in the LatinXChem event (as co-author of the work), 2020;
- Honorable Mention due to Innovative Idea at the Mimesis Hackathon, University of Pernambuco, Brazil, 2020;
- Honorable Mention due to the presented work entitled: “Assessing Peptide Adhesion to Hematite Surface: Towards Biofuel Cell Developments” at the Scientific Computation National Laboratory, Brazil, 2016;
- Travel Grant Award, Institute Pasteur, Uruguay, 2017;
- Travel Grant Award, University of Buenos Aires, 2017;

Complementary Education

- **Protein Engineering with Rosetta: from fundamental principles to tutorial**, Sao Paulo University, 2019
- **Numerical Solutions of PDE with FreeFem++,** Federal University of Pernambuco, 2018
- **Introduction to Italian Language to Academic Purposes**, Federal University of Pernambuco, 2018
- **Measurement of Protein Relaxation Using Nuclear Spin Relaxation**, Buenos Aires University, 2017
- **Multiscale methods from Fundamental Principles to Tutorials**, Sao Paulo University, 2017
- **Performing Molecular Simulations with SIRAH Force Field**, Montevideo Pasteur Institute
- **Biomembranes Protein Simulations**, Scientific Computation National Laboratory, 2016
- **Electronic structure semi-empirical quantum calculations**, Scientific Computation National Laboratory, 2016
- **Modern Techniques in Molecular Simulations**, Sao Paulo University, 2015

- **Membrane Biophysics**, Brazilian Biophysics Society, 2015

Publications (5 Peer-reviewed works and 1 online preprint) H-index: 2, 9 citations.

- Ferraz, MVF; Gonçalves, EM; Coêlho, DF; Wallau, G; Lins RD; Immune evasion of SARS-CoV-2 variants of concern is driven by low affinity to neuatralizing antibodies. **Chemical Communication**, 2021.
- Ferraz, M. V. F., and Lins, R. D. Characterizing Binding Kinetics and Thermodynamics of Computer-designed Nanobodies Targeting SARS-CoV-2 RBD. **Biophysical Journal**, 2021.
- Ferraz, M.V.F, Adan, W.C.S.; Lins, R.D. Unraveling the Role of Nanobodies Tetrad on Their Folding and Stability Assisted by Machine and Deep Learning Algorithms. **Lecture notes in Computer Sciences**, 2020.
- Freire, M.C.L.C.; Silva, Y.A.M.; Ferraz, M.V.F.; Cruz, C.H.B.; Ferreira, L.S.; Pedrosa, M.F.F.; Barbosa, E.G. Molecular Basis of Tityus Stigmurus Alpha Toxin and Potassium Channel Kv1.2 Interactions. **Journal Of Molecular Graphics & Modelling**, V. 87, P. 197-203, 2019;
- Coêlho, D.F.; Ferraz, M.V.F.; Marques, E.T.A.; Lins, R.D.; Viana, I.F.T. The Influence Of Biotinylation On The Ability Of A Computer Designed Protein To Detect B-Cells Producing Anti-HIV-1 2F5 Antibodies. **Journal Of Molecular Graphics & Modellin**g, V. 93, P. 107442, 2019. PC Resende, FG Naveca, RD Lins, FZ Dezordi, MVF Ferraz, EG Moreira, et al. The ongoing evolution of variants of concern and interest of SARS-CoV-2 in Brazil revelaed by convergent indels in the amino (N)-terminal domain of the Spike protein, **MedRxiv**, 2021 (Submitted to the **Emerging Infectious Diseases**)

Invited Talks

- Antibodies – antigens interactions through an atomistic perspective (In portuguese), National Congress of Immunology, Brazil, 2021
- Not all chemists wear a white coat: COVID-19 pandemics in the computation in petaescale era (In portuguese), National Online Congress of Chemistry, Brazil, 2021.
- Protein Engineering in the Interface of Thermodynamics and Machine Learning (In portuguese), CESAR School, Brazil, 2020.
- Impact of STEM within the universities: Zika Virus diagnostic (In portuguese), University Radio, Brazil, 2019.

Oral Presentations

- Ferraz, M.V.F.; Lins, R.D.; Insights into the binding mechanism reveal the molecular selectivity of VHH-72 against SARS-CoV-1 but not for SARS-CoV-2 RBD. In: Biological Diffusion and Brownian Dynamics Brainstorm Meeting 5 (BDBDB), 2021, Heidelberg (Online).
- Ferraz, M.V.F.; Adan, W. C. S.; Coêlho, D. F.; Lins, R. D. Machine Learning Associated with Enhanced Sampling Simulations to Engineering Immunoreactive Proteins. eSSENCE-EMCC Meeting on Multiscale Modelling of materials and molecules in complex systems, Uppsala University, Sweden (Online), 2020.
- Ferraz, M. V. F.; Coêlho, D. F. ; Adan, W. C. S. ; Carvalho, R. D. ; Lins, R. D. . Rational design of a high affinity nanobody binding ZIKV NS1 protein aiming at differential serological diagnostic. IV Advanced School on Biomolecular Simulation: protein engineering with Rosetta, from fundamental principles to tutorial, Brazil, 2019.
- Ferraz, M. V. F.; Lins, R. D. . Adhesion between peptides and mineral surfaces aiming at green energy production. 2nd Protein Biohpysics at the end of world, Argentina, 2017.
- Ferraz, M. V. F.; Viana, I. F. T. ; Lins, R. D. . Characterizing the temperature-dependent conformational transition of dengue virus envelope protein. III Advanced School on Biomolecular Simulation: Multiscale Methods from Fundamental Principles to Tutorials, Brazil, 2017.
- Ferraz, M. V. F.; Lins, R. D. . Assessing the Molecular Basis of Flavivirus Breathing and its Consequence to Antibody Sensitivity. Performing Molecular Simulations with SIRAH force field, Uruguay, 2017.
- Ferraz, M. V. F.; Lins, R. D. . Understanding Hematite Surface Adhering Peptides. II Advanced School on Biomolecular Simulation, Brazil, 2016.

- Ferraz, M. V. F.; Cunha, K. C. ; Coêlho, D. F. ; Lins, R. D. . Assessing the Structural Features of Engineered VHH Antibodies targeting a Recombinant Nucleoprotein of Araucaria Hantavirus. I Advanced School on Biomolecular Simulation, Brazil, 2015.
- Ferraz, M. V. F.; Lins, R. D. . Assessing structural features of VHH-based antibodies used on novel Hantavirus Pulmonary Syndrome diagnosis via molecular dynamics. V STINT Workshop on Understand Biocompatibility of Polymerics Surface, Brazil, 2015.

Lecturing Activities

- **Volunteer High school Teacher**, Gradação Project, Federal University of Pernambuco (2019): Taught physics and chemistry classes at high-school level for needy students to prepare for university entrance exams in Brazil. In the occasion, students with disabilities joined the project.
- **Teacher Assistant**, Post-graduate Chemistry Program, Federal University of Pernambuco (2021): Taught some of the practical and theoretical lessons of the course “Molecular Biophysical Chemistry”.

Committees Membership

- Diploma Work Defense Committee of Julia Gabriela da Silva (Evaluation and reduction of the overweight indicator in the production of PVC tubes by extrusion) Bachelor of Chemical Engineering, Federal University of Pernambuco, 2021.
- Diploma Work Defense Committee of Yamê Cavalcatin Bezerra (Implementing APPC plan in an oil refinery). Bachelor of Chemical Engineering, Federal University of Pernambuco, 2020.
- Poster Jury at the XXIX Scientific Initiation Congress from the Rural Federal Univeristy of Pernambuco, 2019.
- Diploma Work Defense Committee of Larissa Dias da Silva Santos (Design of novel antagonists of the 3-hydroxykynurenine transaminase enzyme: a prototype for a new larvicide). Bachelor of Chemistry, Federal University of Pernambuco, 2019.

Technical Skills

- Programming Languages: C, Python.
- Software Packages: GROMACS; Rosetta; PLUMED; Haddock; Gaussian, MOPAC.
- Mathematical Packages: MATLAB, FreeFem++.
- Computational Methodologies: Machine/Deep Learning; Computational Protein Design; Molecular Dynamics; enhanced sampling in MD simulations (Metadynamics, Umbrella Sampling); Out-of-equilibrium MD simulations (Steered MD, Targeted MD); Force-field parametrization; Quantum-chemical calculations.
- Solid mathematical background.

Languages

- Portuguese (Native)
- English (Full Professional Proficiency, Advanced)
- French (Limited Working Proficiency, Intermediary)