Matheus Ferraz

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RESEARCH PROFILE

Professional with 8 years of experience in scientific research. My portfolio lies in structural bioinformatics and includes simulation of biological macromolecules, especially addressed towards viral infections. In the last years, I have computer-designed proteins against viruses (SARS-CoV-2 and Chinkungunya), predicted pathogen-host interactions in the context of virology and cancer, and virtually screened drugs against viruses and bacteria.

EDUCATION

- Ph.D. Chemistry, Federal University of Pernambuco, Brazil (2019-Present).
  Doctoral stay at the Heidelberg Institute for Theoretical Studies (2021 – Present).
- MSc. Chemistry, Federal University of Pernambuco, Brazil (2018-2019)
- B.Sc. Chemical Engineering, Federal University of Pernambuco, Brazil (2013 – 2018).

RESEARCH TRAINING

- Visiting Ph.D. student, **Heidelberg Institute for Theoretical Studies**, Germany (2021 – Present)
  Advisor: Rebecca C. Wade; Molecular and Cellular Modelling group
  Activities:
  - Calculation of binding kinetics and thermodynamics properties (k_{on}, k_{off}, and k_D) for protein-ligand, protein-protein (nanobodies targeting SARS-CoV-2 RBD; heparin targeting SARS-CoV-2 spike protein) and protein-peptide complexes (MHC Class I – peptides)
  - Drug design via generative neural network models

- Ph.D. student, **Federal University of Pernambuco**, Brazil (2019 – Present)
  Advisor: Roberto D. Lins; Department of Fundamental Chemistry and

- Ph.D. student collaborator, **Oswaldo Cruz Foundation**, Brazil (2019 – Present)
  Advisor: Roberto D. Lins; Biomaterial modelling group, Department of Virology
  Activities:
  Drug discovery and design; computational design of proteins against viral infections (Zika virus, Coronavirus); free energy calculations via enhanced sampling simulations; machine learning development to compute protein – protein binding free energies; member of the Brazilian COVID-19 genomic surveillance team at FIOCRUZ.

- Undergraduate Scientific Initiation, **Oswaldo Cruz Foundation**, Brazil (2015 – 2018)
  Advisor: Roberto D. Lins; Biomaterial modelling group, Department of Virology
  Activities:
  - Modelling of peptide – mineral surfaces interactions using molecular dynamics, metadynamics, and steered MD; modelling of camelid nanobodies.

- Undergraduate Diploma work, **Federal University of Pernambuco**, Brazil (2017-2017)
  Advisor: Sérgio Lucena; Laboratory for Advanced Control and Processes Optmization, Department of Chemical Engineering
  Activities:
  - Modelling of biochemical processes via SuperPro Designer®.

PUBLICATIONS

1. **Ferraz, M.V.F.,** Viana, I.F.T., Coêlho, D.F., Cruz, C.H.B., Lima, M.A., Aragão, M.A.L., Lins, R.D. Association strength of E6 to E6AP/p53 correlates with HPV-mediated oncogenesis risk. **Biopolymers**, 2022
2. Matos, I.A.; Pinto, A.C.G.; **Ferraz, M.V.F.**, Adan, W.C.S.; Rodrigues, R.P.; Santos, J.X.; Kitagawa,R.R.; Lins, R.D.; Oliveira, T.B. and Costa, N.B. Identification of potential *Staphylococcus aureus* dihydrofolate reductase inhibitors using QSAR, molecular docking, dynamics simulations and free energy calculation. **Journal of Biomolecular Structure and Dynamics**, 2022.
3. Naveca, Felipe Gomes; Nascimento, Valdinete; Souza, Victor; Corado, André De Lima; Nascimento, Fernanda Silva, George Mejía, Matilde Contreras Brandão, Maria Júlia Costa, Ágatha Duarte, Débora Pessoa, Karina Jesus, Michele Gonçalves, Luciana Fernandes, Cristiano Mattos, Tirza Abdalla, Ligia Santos, João Hugo Martins, Alex Chui, Fabiola Mendonça Val, Fernando Fonseca De Melo, Gisely Cardoso Xavier, Mariana Simão Sampaio, Vanderson De Souza Mourão, Maria Paula Lacerda, Marcus Vinícius , Batista, Érika Lopes Rocha Magalhães, Alessandro Leonardo Álvares Dábilla, Nathânia Pereira, Lucas Carlos Gomes Vinhal, Fernando Miyajima, Fabio Dias, Fernando Braga Stehling Dos Santos, Eduardo Ruback; Coêlho, Danilo; **Ferraz, M.V.F.;** Lins, Roberto; Wallau, Gabriel; Luz Delatorre, Edson; Gräf, Tiago; Siqueira, Marilda; Mendonça Resende, Paola Cristina Bello, Gonzalo ; Spread of Gamma (P.1) Sub-Lineages Carrying Spike Mutations Close to the Furin Cleavage Site and Deletions in the N-Terminal Domain Drives Ongoing Transmission of SARS-CoV-2 in Amazonas, Brazil. **Microbiology Spectrum**, 2022. (Article)
4. **Ferraz, M.V.F.**; Gonçalves, E.M; Coêlho, D.F; Wallau, G.; Lins R.D.; Immune evasion of SARS-CoV-2 variants of concern is driven by low affinity to neutralizing antibodies. **Chemical Communication**, 2021 (Article)
5. Resende, P.C., Naveca, F.G., Lins R.D., Dezordi F.Z., **Ferraz, M.V.F.**, Moreira, E.G., 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, **Virus evolution**, 2021 (Article)
6. **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. (Book chapter)
7. 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; (Article)
8. 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. (Article)

SUBMITTED PUBLICATIONS

1. **Ferraz, M.V.F.**; Cláudio, J.; Lins, R.D.; Teixeira, E.S. Artificial neural networks to predict structure-based protein-protein free energy of binding from Rosetta-calculated properties. Submitted to Journal of Chemical Information and Modeling. (Article) – Available on the Preprint
2. Maciel, L.G.; **Ferraz, M.V.F**.; Oliveira, A.A.; Guido, R.V.C.; Lins, R.D.; Anjos, J.A.; Soares, T.A. The X-ray structure of the 3-hydroxykynurenine transaminase from *Aedes aegypti*: a novel target to combat the transmission of arboviruses. Submitted to RSC Medicinal chemistry journal (Article)

MANUSCRIPTS IN PROGRESS

1. **Ferraz, M.V.F**; Adan, W.C.S.; Viana, I.F.T; Wade, R.C.; Lins, R.D. A data-centric and enhanced sampling-based approach to the design of artificial nanobodies. (Article)
2. Lima, T.E; **Ferraz, M.V.F**.; Brito, C.A.A; Ximenes, P.A.; Mariz C.A.; Lins, R.D.; Viana, I.F.T. Assessment of the IgG antibody profile of individuals infected with SARS-CoV-2 and determination of serological prognostic markers for disease severity. (Article)
3. Adan, W.C.S; **Ferraz, M.V.F**.; Lins, R.D. Assessing the dynamical variability and affinity of VHH antigen-binding loops by sampling their conformational ensemble. (Article)
4. Purificação, A.F.; **Ferraz, M.V.F**; Freire, M.C.L; Viana, I.F.T; Lins, R.D. Design of a synthetic protein targeting Chikungunya virus E2B domain epitopes towards acute phase diagnostics and therapy.

TECHNICAL SKILLS

- Programming Languages: Python
- Amazon web service (AWS); Git; Notions of structured query language (SQL)
- Computational Methodologies: Drug discovery and design; 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); Brownian Dynamics; τ-random accelerated MD; Quantum-chemical calculations.
- Solid mathematical background.

FELLOWSHIPS

- Research Grants-Bi-nationally Supervise DoctoralDegrees/Cotutelle, Deutscher Akademischer Austauschdienst, DAAD, Germany, 2021
- Doctoral Scholarship, 142297/2019-4, National Council for Scientific and Technological Development CNPq, Brazil, 2019
- Master Scholarship, National Council for Scientific and Technological Development, CNPq, Brazil, 2018
- Technical Cooperation scholarship, Foundation for Scientific Affairs from Pernambuco, FACEPE, Brazil, 2016
- Scientific Initiation, Coordination for the Improvement of higher education, CAPES, Brazil, 2015

AWARDS

- Honorable mention at the LatinXchem, American Chemical Society
- Honorable Mention due to Innovative Idea at the Mimesis Hackathon, University of Pernambuco, Brazil, 2020;
- Travel Grant Award, Institute Pasteur, Uruguay, 2017;
- Travel Grant Award, University of Buenos Aires, 2017;
- 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;

REFEREE ASSISTANT FOR SCIENTIFIC JOURNAL

- Journal of molecular recognition - Wiley online library

INVITED TALKS

- Computer simulations in the fight of viral infections (In Portuguese), National Online congress of multidisciplinary sciences, Brazil, 2022
- Biomolecular modeling and artificial intelligence in drug and therapeutic proteins discovery (In Portuguese), National Online congress of genetics and molecular biology, Brazil, 2022
- Protein design to fight COVID-19: opportunities in health within engineering (In Portuguese), Department of Chemical Engineering, Federal University of Pernambuco, 2021
- Antibodies – antigens interactions through an atomistic perspective (In portuguese), National Online 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 as a strategy against COVID-19 (In Portuguese), VI Chemistry school of the Federal University of Sergipe, 2020.
- 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), Federal University of Pernambuco Radio, Brazil, 2019.

CONFERENCES – ORAL PRESENTATIONS (selected)

- **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.

ABSTRACTS PUBLISHED IN CONGRESSES (selected)

- **Ferraz, M.V.F**; Adan, W.C.S; Viana, I.F.T.; Wade, R.C.; Lins, R.D. Structure-based computational design of nanomolar-binding VHHs targeting the SARS-CoV-22 spike protein. In: Flagship Initiative Engineering Molecular Systems Young Scientist Retreat, 2022, Dannenfels. Abstract Booklet, 2022. p. 20-20.
- **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. V Biological Diffusion and Brownian Dynamics Brainstorm Meeting, 2021. p. 11-11
- **Ferraz, M.V.F**; Seitz, C.; Lins, R.D. Probing the Conformational Dynamics of a Conserved Epitope in the SARSCoV-1 and -2 Spike Protein Using Gaussian Fluctuations and Collective Motions. In: Workshop on Computer Simulation and Theory of Macromolecules, 2021, Hünfeld. Abstracts of poster contributions, 2021. p. 34-34.

TEACHING EXPERIENCE

- **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” under the supervision of Danilo F. Coêlho.
- **Teacher Assistant**, Undergraduate Chemistry Program, Federal University of Pernambuco (2019): Taught lectures on “Introductory chemistry” to the undergraduate-level in chemistry major under the supervision of Prof. Ricardo Oliveira.
- **Minicourse,** Molecular modeling of antigen-antibodies (In Portuguese), National Online Congress of Immunology, 2022.
- **Minicourse,** Molecular modeling in biotechnology (In Portuguese), Oswaldo Cruz Foundation 2022
- **Minicourse**, Molecular dynamics: Theory and applications in biotechnology and health (in Portuguese), Oswaldo Cruz Foundation, 2021.

COMITTEE PARTICIPATION (All the Works in Portuguese)

- Diploma Work Defense Committee of Júlia Silvestre de Sena. (Supervision and control of a process in a industry of powder detergent) Bachelor of industrial chemistry, Federal University of Pernambuco, 2022.
- Diploma Work Defense Committee of Vinícius Firmino dos Santos (Computational simulation of nucleotides adsorption of polymeric brushes of poly(dimethylaminoethyl acrylate) Bachelor of Chemistry, Federal University of Pernambuco, 2021.
- Diploma Work Defense Committee of Isabelle Cristine de Lima (Application of the Kano and PDCA method on the assessment of quality service of the Stone Pagamentos S.A.) Bachelor of Chemical Engineering, Federal University of Pernambuco, 2021.
- 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.
- 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.
- Poster Jury at the XXIX Scientific Initiation Congress from the Rural Federal University of Pernambuco, 2019.

OUTREACH AND NEWS

- http://cfq.org.br/noticia/condequi-encerra-com-temas-sobre-educacao-pesquisa-e-sustentabilidade/ (Brazilian Federal Chemistry Council, in Portuguese, 2021)
- https://www.youtube.com/watch?v=lIZMuCG2qf0 (Discovery channel documentary – Brazil science, episode 3: supercomputer, In Portuguese, 2016)

LANGUAGES

- Native Portuguese
- Fluent English
- Advanced German

REFERENCES

Prof. Dr. Rebecca Wade
Heidelberg Institute for Theoretical Studies, Germany
e-mail: rebecca.wade@h-its.org

Prof. Dr. Roberto Lins
Aggeu Magalhães Institute, Brazil
e-mail: roberto.lins@cpqam.fiocruz.br

Prof. Dr. Thereza Amélia Soares
Universidade de São Paulo, Brazil
e-mail: thereza.soares@usp.br

Prof. Dr. Ariane Ferreira Nunes Alves
Technische Universität Berlin, Germany
e-mail: ferreira.nunes.alves@tu-berlin.de