Diego Enry Barreto Gomes, PhD
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Professional Summary

Research scientist and scientific-software engineer with 15+ years at the interface of computation and research infrastructure. Lead developer of VMD 2.0 (Visual Molecular Dynamics), specializing in high-performance file I/O, GPU acceleration, and portability across CPU/GPU architectures (C/C++, Python, CUDA), proven on NVIDIA Grace Hopper/Blackwell HPC systems. Deep hands-on experience managing and optimizing HPC resources and cluster administration, SLURM/PBS, compilation and benchmarking of molecular-mechanics and quantum-chemistry codes — together with machine learning for scientific data (scikit-learn, free-energy prediction) and reproducible engineering practice (version control, testing, packaging, containerization). Background spanning computational chemistry, biophysics, and bioinformatics, with two French postdocs (Strasbourg, ENS-Cachan) and a career built on training researchers and bridging computational and experimental teams.

Professional experience:

Research Scientist - Auburn University – Department of Physics - 07/2021 – Current

- Software development for molecular dynamics simulation applications
    - Visual Molecular Dynamics 2 (VMD2) - My work centers on high-performance file I/O and analysis for very large biomolecular systems, including an individually developed suite of molfile readers and the WaterCompress trajectory codec, alongside co-developed accelerations of molecular-surface generation, secondary-structure assignment, and glycan rendering.
    - CyberShuttle (https://cybershuttle.org) - Cybershuttle expertly balances local and remote computing, by orchestrating tasks and data between machines. Schedule time-sensitive, small tasks locally, and reserve compute-intensive tasks for powerful remote HPC resources, with data transparently accessible everywhere
    - DARPA Nodes project - nodeskit: a toolkit to find and retrieve structures for InterPro families, fetch annotations, repair structures, and prepare molecular dynamics simulations; deployed on the OLCF Frontier supercomputer, targeting 10,000+ one-microsecond simulations of proteins from diverse families towards a new protein language and network model to predic function from sequence.
- Mechanobiology of bacterial adhesins
- Mechanical anisotropy Nanobodies and Affibodies of biotechnological interest
- NVIDIA-DGX cluster management

Visiting Professor – Department of Computer Sciences - Federal University of Juiz de Fora (Brazil) - 03/2019 – 03/2021

- Graduate School Teaching:
    - 60h - Molecular Modelling for Computational Scientists
    - 60h - Bioinformatics for Computational Scientists
- Supervised MLOps optimization of machine learning workloads.
- Supervised the development of ML models for predicting binding free energies of Host-Guest systems.

Post-doctoral fellow at University of Strasbourg (France) - 12/2016 – 03/2019

- Development of a HPC cheminformatics framework (ChemFlow)
- Led to the discovery of five Smooth Muscle Myosin 2 inhibitors.
- Contributed with quantum chemistry charge-parametrization of the French National Chemical Library.

Principal Investigator at INMETRO (National Institute of Standards - Brazil) - 11/2011 – 12/2018

- Founded and managed the Computational Biology Laboratory.
    - Established a computational biology platform to function as a contract research organization (CRO).
- Secured funding through CNPq (PROMETRO 2012-2015) and Co-PI CAPES (Computatonal Biology 2015-2019).
- Supervised graduate and undergraduate students.

Assistant Professor (contract) – Federal University of Rio de Janeiro (Brazil) - 03/2012 – 03/2014

- Undergraduate School
    - 60h – Structural Biology and Drug Discovery (XBQ352 - Biotechnology)
    - 75h - Bioinformatics (XBT350 - Biotechnology)
    - 60h – Bioinformatics I (CFB222 - Biophysics)
    - 60h – Host-guest interactions (BMB428 - Biophysics)
    - 90h – Bioinformatics and Molecular Modeling (BMB413 - Biophysics)

Post-doctoral fellow at ENS Cachan (France) - 08/2010 – 07/2011

- Developed a genetic algorithm for protein-protein docking.
- Implemented a HPC pipeline to integrate computational chemistry tools and generate syntetic reports.

Software & Programing Skills

Experienced: BASH, Python, Fortran77/90, Slurm and PBS schedulers.
Eventual user: C/C++ Awk, TCL-TK, KNIME, Rdkit.
Experienced: VMD, NAMD, AMBER, GROMACS, CHARMM +, PyMol.
User only: Gaussian, GAMESS and NWChem.

Research Interests

High Performance Computing for research, Computational Biophysics and Computational Chemistry applied to: Biofuels, Nanosensors, Proteins in nanomaterials, Proteins in non-aquous solvents, Protein Structure & Drug Design, Virtual Screening, Protein-Protein Docking

Current High-Performance Computing Allocations

Over two decades of continuous use of high-performance computing for research — from early Brazilian grid platforms (BioPAUÁ) and the Pacific Northwest National Laboratory to U.S. national infrastructure (NSF ACCESS, formerly XSEDE) and TACC — including preparing and managing competitive allocation requests and coordinating simulation-hour usage across research teams. Recent allocations on NSF:

- **Principal Investigator** — BIO250212: Investigating Hydrogen Mass Repartitioning in Steered Molecular Dynamics Simulations of the SdrG Adhesin–Fibrinogen Complex.
- **Principal Investigator** — BIO230132: Mechanical Anisotropy of the PD-L1–Affibody Complex.
- **Allocation Manager** — BIO240250: Evolution of the Mechanostability of Bacterial Adhesins.

Academic Background

2006 - 2010 PhD (Biophysics).

Instituto de Biofísica Carlos Chagas Filho - Universidade Federal do Rio de Janeiro, Brazil
& Pacific Northwest National Laboratory – USA.
Thesis: Molecular Models to Confine Organophosphorous Hydrolase in Nanostructures
Supervisors: Dr. Pedro Geraldo Pascutti (UFRJ) & Dr. Thereza Amélia Soares (PNNL)

2004 – 2006: Master of Science (Biological Sciences - Biophysics).

Instituto de Biofísica Carlos Chagas Filho - Universidade Federal do Rio de Janeiro, Brazil
Dissertation: Study of Falcipain-2 in Complex with Ligands by Molecular Modeling and Dynamics to Support Antimalarial Rational Drug Design.
Supervisor: Dr. Pedro Geraldo Pascutti

2000 - 2004 Bachelor of Science (Biological Sciences – Medical Modality)

Universidade Federal do Rio de Janeiro, UFRJ, Rio De Janeiro, Brazil

Recent complementary formation

2024 – Princeton University
July - INTERSECT Research Software Engineering Bootcamp (36h)

2024 - National Center for Supercomputing Applications
- March - Intro to Apptainer Workshop (2h)
- April - Advanced Apptainer Workshop (8h)

2023 - San Diego Supercomputer Center (Summer Institutes)
- August - HPC and Data Science Summer Institute (40h)
- July - Cyberinfrastructure-Enabled Machine Learning (CIML) (40h)

2023 – Nvidia Deep Learning Institute
- January - Fundamentals of Deep Learning (8h)
- March - Data Parallelism: How to Train Deep Learning Models on Multiple GPUs (8h)

2019 – Global July Program – Universidade Federal de Juiz de Fora.
- July - Python For Bioinformatics (30h)
- Exploring protein sequence and functional information (3h)
- Introduction to Molecular Dynamics and the ACPYPE (4h)

2018 - Enhanced Sampling Workshop – University of Illinois at Urbana-Champaign.
- 20h - Theory Enhanced sampling techniques
- 20h - Practice Enhanced sampling techniques

Pre-print articles

- **Gomes, DEB;** Melo, MCR; Gomes, PSFC; Bernardi, RC. *Bridging the gap between in vitro and in silico single-molecule force spectroscopy*. Bioarxv. doi: 10.1101/2022.07.14.500151

Peer-reviewed articles by category

Cyberinfrastructure and Databases

Marru, S; Pierce, M; Plale, B; Pamidighantam, S; Wannipurage, D; Christie, M; Ranawaka, I; Abeysinghe, E; Quick, R; Tajkhorshid, E; Koric, S; Basney, J; Spivak M; Isralewitz B; Bernardi R; **Gomes D**; Krishnan G; Bazhenov M; Smallen S; Majumdar S; Arkhipov A, Dai K; Liu, Xiao-Ping. *Cybershuttle: An end-to-end Cyberinfrastructure Continuum to accelerate Discovery in Science and Engineering*. PERC '23 - Practice & Experience in Advanced Research Computing. 2023. doi: 10.1145/3569951.3593602

Gomes D.E.B ; Galentino K; Sisquellas M; Monari L; Bouysset C; Cecchini M. ChemFlow-From 2D Chemical Libraries to Protein–Ligand Binding Free Energies. Journal of Chemical Information and Modeling 2023.doi: 10.1021/acs.jcim.2c00919

Naranjo-Feliciano D, Izquierdo-Alvarez L, Calero-Ramos R, Hernández-Alvarez L, Bouza-Figueroa J, **Gomes DEB**; Valiente PA, Calvet HAC, Pacutti PG. *A molecular docking integrated platform for virtual screening of bioactive compounds*. Biotecnologia Aplicada. **2021**; 38(3):3211-3217.

Cerdan AH, Sisquellas M, Pereira G, **Gomes DEB**, Changeux JP, Cecchini M. **2020**. *The Glycine Receptor Allosteric Ligands Library (GRALL)*. Bioinformatics, doi:10.1093/bioinformatics/btaa170

Silva, Alan, Osthoff, Carla, Oliveira, Cristiane, **Gomes, D. E. B.**, Hill, E., Dardenne, L. E., Barros, P. M., Loureiro , P. A. A .G. L., Novaes, R, Pascutti, P G. The BioPAUÁ Project: A Portal for Molecular Dynamics Using Grid Environment. Lecture Notes in Computer Science. v.3594, p.214 - 217, 2005.

Machine Learning and Artificial Intelligence

Melo MC; **Gomes D.E.B.**; Bernardi R.C. *Molecular Origins of Force-Dependent Protein Complex Stabilization during Bacterial Infections*. JACS - Journal of the American Chemical Society 2023. doi:10.1021/jacs.2c07674

Gomes, P. S. F. C., **Gomes, D. E. B.,**; Bernardi, R. C. *Protein structure prediction in the era of AI: Challenges and limitations when applying to in silico force spectroscopy*. Frontiers in Bioinformatics. **2022**;(2). doi:10.3389/fbinf.2022.983306

Carvalho, Ruan M. ; Rosa, Iago G. L. ; Goliatt, Priscila V. Z. C. ; **Gomes, Diego E. B.** ; Goliatt, Leonardo. *Prediction of Cyclodextrin Host-Guest Binding Through a Hybrid Support Vector Method*. Advances in Intelligent Systems and Computing. 1ed.: Springer Singapore, (2021) v. , p. 309-317. doi: 10.1007/978-981-16-1543-6_30

Carvalho, RM. ; Rosa, IGL. ; **Gomes, DEB**. ; Goliatt, PVZC ; Goliatt, L. *Gaussian processes regression for cyclodextrin host-guest binding prediction*. Journal of Inclusion Phenomena and Macrocyclic Chemistry, v. 101, p. 149-159, 2021. doi; 10.1007/s10847-021-01092-4

Montalvo-Acosta JJ, Pacak P. **Gomes DEB**, and Cecchini M. **2018**. *A Linear Interaction Energy Model for Cavitand Host–Guest Binding Affinities*. The Journal of Physical Chemistry B, doi: 10.1021/acs.jpcb.8b03245.

MechanoBiology

Chantraine C, Priscila S. F. C. Gomes P.S.F.C, Mathelié-Guinlet M, and **Gomes D.E.B.**, Zheng Z, Clowry J, Turley M.B., Irvine A.D., Geoghegan J.A., Bernardi R.C., Dufrêne Y. F. Ultrastrong. *Staphylococcus aureus adhesion to human skin: Calcium as a key regulator of noncovalent interactions*. Science Advances 2025. Doi: 10.1126/sciadv.adu7457

Natividade, R.S.; Koehler M, Gomes P.S.F.C., Simpson J.D., Smith, S.C., **Gomes D.E.B.**, de Lhoneux J., Yang J., Ray A, Dermody T.S., Bernardi R.C., Ogden, K. M., Alsteens D. *Deciphering molecular mechanisms stabilizing the reovirus binding complex*; PNAS - Proceedings of the National Academy of Sciences of the United States of America 2023. doi: 10.1073/pnas.2220741120

Gomes, Priscila S. F. C.; Forrester, Meredith; Pace, Margaret; **Gomes, Diego E. B.**; Bernardi, Rafael C. May the force be with you: The role of hyper-mechanostability of the bone sialoprotein binding protein during early stages of Staphylococci infections. Frontiers in Chemistry 2023 doi: 10.3389/fchem.2023.1107427

Nanomaterials

Gomes, D. E. B., Lins, R. D., Pascutti, P. G., Lei, C., Soares, T.A.; *Conformational Variability of Organophosphorus Hydrolase upon Soman and Paraoxon Binding*. Journal of Physical Chemistry. B. , v.115, p.15389 - 15398, 2011. doi: 10.1021/jp208787g

Gomes, D. E. B., Lins, R. D., Pascutti, P. G., Lei, C., Soares, T. A. *The Role of Nonbonded Interactions in the Conformational Dynamics of Organophosphorous Hydrolase Adsorbed onto Functionalized Mesoporous Silica Surfaces*. Journal of Physical Chemistry. B. , v.114, p.531 - 540, 2010. doi: 0.1021/jp9083635

Gomes, D. E. B., R. D. Lins, Pascutti, P. G., Straatsma, T.P., Soares, T. A. *Molecular Models to Emulate Confinement Effects on the Internal Dynamics of Organophosphorous Hydrolase*. Lecture Notes in Computer Science. v.5167, p.68 - 78, 2008. doi: https://doi.org/10.1007/978-3-540-85557-6_7

Biomembranes and Local Anesthetics

Bernardi, R. C., **Gomes, D. E. B.**, Gobato, R., Taft, C. A., Ota, A. T., Pascutti, P. G. *Molecular dynamics study of biomembrane/local anesthetics interactions*. Molecular Physics, v.107, p.1437 - 1443, 2009. doi: 10.1080/00268970902926238

Bernardi, R. C., **Gomes, D. E. B.**, Ito, A. S., Ota, A. T., Pascutti, P. G., Taft, C. *Density functional and molecular dynamics simulations of local anesthetics in 0.9% NaCl solution*. Molecular Simulation. v.33, p.1135 - 1141, 2007. doi: 10.1080/08927020701620636

Bernardi, R. C., **Gomes, D. E. B.**, Pascutti, P. G., Ito, A. S., Taft, C. A., Ota, A. T. *Water solvent and local anesthetics: A computational study*. International Journal of Quantum Chemistry. v.107, p.1642 - 1649, 2007. doi: 10.1002/qua.21300

Bernardi, R. C., **Gomes, D. E. B.**, Pascutti, P. G., Ito, A. S., Ota, A. T. *Theoretical studies on water-tetracaine interaction*. International Journal of Quantum Chemistry. v.106, p.1277 - 1282, 2006. doi: 10.1002/qua.20881

Drug Discovery for Neglected Diseases

Hernández González, J. E., Salas-Sarduy, E., Hernández Alvarez, L., **Gomes, D.E.B.**, Pascutti, P. G., Oostenbrink, C., & Leite, V. B. P. *In silico identification of noncompetitive inhibitors targeting an uncharacterized allosteric site of falcipain-2.* Journal of Computer-Aided Molecular Design, **2021**;*35*(10),1067–1079. doi:10.1007/s10822-021-00420-7

Hernández L.A., Hernández J.E.G., **Gomes, D.E.B.**, Pascutti PG. *Dissecting a novel allosteric mechanism of cruzain: a computer-aided approach.* **2019**. PLOS One 14(1). doi:10.1371/journal.pone.0211227

Hernández L.A., Naranjo F.D., Hernández J.E.G., Soares R.O., **Gomes, D.E.B.**, Pascutti PG. Insights into the Interactions of Fasciola hepatica Cathepsin L3 with a Substrate and Potential Novel Inhibitors through in Silico Approaches. PLoS Neglected Tropical Diseases. v.9, p.e0003759, **2015**. doi: https://doi.org/10.1371/journal.pntd.0003759

Antibody Engineering

Gomes D.E.B., Yang B, Vanella R., Nash M., Bernardi R. *Integrating Dynamic Network Analysis with AI for Enhanced Epitope Prediction in PD-L1:Affibody Interactions.* Journal of the American Chemical Society **2024** 146 (34), 23842-23853 doi: 10.1021/jacs.4c05869

Yang, B, **Gomes D.E.B**, Liu Z, Santos M.S., Li J, Bernardi R.C., Nash M.A. *Engineering the Mechanical Stability of a Therapeutic Complex between Affibody and Programmed Death-Ligand 1 by Anchor Point Selection.* ACS Nano ***2024*** *18 (46), 31912-31922. doil: 10.1021/acsnano.4c09220*

Bioenergy

Vieira, I. P. v., Cordeiro, G. T., Gomes, D. E. B., Melani, R. D., Vilela, L. F., Domont, G. B., Mesquita, R. D., Eleutherio, E. C. A., & Neves, B. C. *Understanding xylose isomerase from Burkholderia cenocepacia: insights into structure and functionality for ethanol production.* **2019**. AMB Express, *9*(1), 73. doi:10.1186/s13568-019-0795-4

Lectures

NAMD/VMD – 64st Computational Biophysics Workshop. Auburn University, AL.
https://www.ks.uiuc.edu/Training/Workshop/Auburn2026/

- VMD 2.0 Features, Performance and Capabilities (27/06/2026)
- How to Produce High-Quality Images with VMD (27/06/2026)

CECAM - EcoCompute 2026, Swiss National Supercomputing Centre, Lugano, Switzerland.
https://www.cecam.org/workshop-details/ecocompute-building-sustainable-scientific-computing-practices-through-academia-industry-collaboration-1475

- Efficient Structural Biophysics at Scale: Accelerating Analysis and Compressing Trajectories in VMD 2.0 (06/06/2026)

Institut de Biologie Physico-Chimique, Paris, France

- VMD 2.0 - Advancing Biomolecular Visualization & Dynamics for Next-Generation Structural Biophysics (21/04/2026)

BPS 2026 (Biophysical Society Annual Meeting), San Francisco, CA

- From structure to motion: Next-generation biomolecular visualization with VMD 2.0. (02/25/2026)

ACS Fall 2025 - American Chemical Society, Washington, DC

- VMD 2.0: Enhancing molecular visualization, dynamics, and structural analysis tools for Biomolecular studies. (08/19/2025)

NAMD/VMD – 63st Computational Biophysics Workshop. Auburn University, AL.
https://www.ks.uiuc.edu/Training/Workshop/Auburn2025/

- VMD 2.0 Features, Performance and Capabilities *(06/08/2025)*
- Cybershuttle for Protein Modeling *(06/08/2025)*
- How to Produce High-Quality Images with VMD *(06/08/2025)*

NAMD/VMD – 62st Computational Biophysics Workshop. Auburn University, AL.
https://www.ks.uiuc.edu/Training/Workshop/Auburn2024B/

- What is new in VMD 2.0 *(16/12/2024)*
- Cybershuttle for Protein Modeling *(18/12/2024)*
- Cybershuttle for Molecular Dynamics Applications *(18/12/2024)*
- How to Produce High-Quality Images with VMD *(18/12/2024)*

NAMD/VMD – 61st Computational Biophysics Workshop. Auburn University, AL.
https://www.ks.uiuc.edu/Training/Workshop/Auburn2024/

- *Introduction to VMD 2.0 (06/24/2024)*
- *How to Produce High-Quality Images with VMD - (06/24/2024)*
- *Cybershuttle for Protein Modeling - (06/28/2024)*

NAMD/VMD – 60th Computational Biophysics Workshop. Auburn University, AL.

- *Ab initio protein structure modeling with Alphafold in VMD (07/17/2023)*

Beckman Institute, University of Ilinois at Urbana-Champaign, IL.

- Mechanical Anisotropy of PD-L1-Affibody Complex Revealed by Single-Molecule Force Spectroscopy and MulEscale Adhesion Analysis (05/22/2023)

Gordon Center for Integrative Science, University of Chicago, IL.

- QwikFold, and why do we still need Modeller? *(08/11/2022)*

Instituto de Biodiversidade e Sustentabilidade, UFRJ-Macaé, Brasil.

- *ChemFlow – From 2D chemical libraries to protein-ligand binding free energies in a few clicks. (09/20/2019)*

Department of Computational Engineering - UFJF – Juiz de Fora, Brasil

- Molecular Modeling for drug discovery & design: Biophysical and Computational Challenges. (05/02/2019)

Laboratório Nacional de Computação Científica – LNCC – Petrópolis – Brazil

- High Throughput Computational Chemistry. (08/24/2018)

Laboratório Nacional de Computação Científica – LNCC – Petrópolis – Brazil

- The MM-PBSA method for estimating binding free energies. (08/26/2016)

Instituto Nacional de Metrologia, Qualidade e Tecnologia, Duque de Caxias, RJ – Brazil

- Accelerating Normal Mode Analisys for Large Biological Macromolecules. Gomes, D. E. B., Perahia, D. (03/14/2014)

Beckman Institute for Advanced Science and Technology - Champaign, IL – USA

- New approaches for biofuel production. (2014)

Workshop da Pós Graduação em Biossistemas - Universidade Federal do ABC - Santo André, Brazil

- A new method for a Fully Flexible Protein-Protein Docking. (2012)

XVIIe congrès du Groupe de Graphisme et Modélisation Moléculaire - La Rochelle – France

- Protein-Protein docking using normal modes and genetic algorithm (2011)

Collège Universitaire Franco-Brésilien Santos Dumont - ENS-Cachan, France.

- Development of a Fully Flexible Protein-Protein Docking Method combining Normal Modes and Genetic Algorithm. *Gomes, DEB, Bisch, PM, Perahia, D, (01/12/2012).*

Third Brazilian Symposium on Bioinformatics, BSB 2008 - Santo André, Brazil

- Molecular Models to Emulate Confinement Effects on the Internal Dynamics of Organophosphorous Hydrolase. Gomes, D. E. B., R. D. Lins, Pascutti, P. G., Straatsma, T.P., Soares, T. A. (2008)

Pacific Northwest National Laboratory - Richland, WA – USA

- ***Attempting to investigate the effects of confinement on Organophosphorus Hydrolase from P. diminuta by Molecular Dynamics simulation.*** Gomes, D. E. B., Soares, T. A., Straatsma, T.P. (2006)

Short-term Courses Ministred

Gomes, DEB (2023)
60th Computational Biophysics Workshop - www.tcbg.illinois.edu/Training/Workshop/Auburn2023/
2h - Ab initio protein structure modeling with Alphafold in VMD

Gomes, DEB (2018)
9th Molecular Modeling School in Biological Systems - www.emmsb.lncc.br
12h - Molecular Dynamics Simulations

Gomes, DEB, Fernandes T. V, Soares, R. Bernardi , R (2016)
8th Molecular Modeling School in Biological Systems - www.emmsb.lncc.br
12h - Basic Molecular Dynamics Simulations

Ritchie, David ; da Silva, M. L. ; **Gomes, D. E. B.** (2014)
7th Molecular Modeling School in Biological Systems - www.emmsb.lncc.br
9h - Protein-Protein Docking & Protein Structural Alignment and Classification.

Gomes, D. E. B., Silva, M. L. (2013).
Instituto Nacional de Metrologia, Qualidade e Tecnologia
12h - Introduction to Metagenomics

Gomes, D. E. B., Pascutti, P.G. (2013).
Instituto de Biofísica Carlos Chagas Filho, Universidade Federal do Rio de Janeiro
90h - Programming applied to Molecular Modeling & Dynamics (Fortran & Bash)

Gomes, D. E. B., Caffarena, E.R. (2012)
6th Molecular Modeling School in Biological Systems - www.emmsb.lncc.br
20h - Practical Molecular Dynamics

Gomes, D. E. B., Pascutti, Pedro G. (2012)
6th School in Nanoscience and Nanotechnology (UFRJ) - http://www.escolanano.org/
12h - Theory & Practice in Computational Nanotechnology

Gomes, D. E. B., Fernandes, T. V. A. (2008)
4th Molecular Modeling School in Biological Systems - www.emmsb.lncc.br
20h - Introduction do Molecular Dynamics

Gomes, D. E. B., Pascutti, P. G. (2004)
IX Semana da Física – Universidade Estadual do Paraná, Londrina, PR - Brazil
4h - Introduction to Molecular Modeling and Dynamics.
12h - Modelling and Dynamics of Biomolecules.

Participation in Examination Boards

1 - Philosophiae Doctor (Biotecnology)
Centro de Biotecnologia - Universidade Federal da Paraíba, ***2021***.
Candidate: Elson José Ferreira Chaves

Thesis: Obtenção de inibidores da subunidade catalítica da ricina, RTA, utilizando métodos de modelagem molecular
Jury:

2 - Philosophiae Doctor (Biologia Computacional e Sistemas)
Instituto de Oswaldo Cruz - Fundação Oswaldo Cruz, 2015
Candidate: Artur Antônio Melo de Lira Brandt
Thesis: Análise da Dissociação entre as proteiínas H-2 de Classe I e Epítopos da Extensão COOH-Terminal da CPB de Leishmanial (L.) Amazonensis.
Jury: Cafarena E. R, Alves C.R., Gomes, D. E. B., Passetti F.

3 - Philosophiae Doctor (Chemistry)
Instituto de Química - Universidade Estadual de Campinas, 2015
Candidate: Tatiana Mello da Costa Faro.
Thesis: Nanoestruturas de Carbono para o Armazenamento de Hidrogênio: Estudos Computacionais.
Jury: Skaf, M. S., Sonoda, M. T., Gomes, D. E. B., Custodio, R., Silva, R. A. N., Vazquez, P. A. M., Mazali, I. O., Gomes, T. C. F.

4 - Master of Science (Information Engineering)
Centro de Matemática, Computação e Cognição - Universidade Federal do ABC, 2013
Candidate: Denis Lucas Silva.
Dissertation: Estudo de padrões em proteínas virais humanas e a sua correlação com a rede de interação dessas proteínas.
Jury: Scott, L.P.,Nascimento, M.Z., Marietto, M.G.B., Honório, K.M., Kamiensky, C.A., Gomes, D.E.B.

5 - Bachelor of Science (Biological Sciences – Medical Modality)
Universidade Federal do Rio de Janeiro, 2021
Candidate: Nilton Silva Júnior
Dissertation: Estudo computacional da dinâmica de interação e seletividade membranar do peptídeo antimicrobiano Psd1

5 - Bachelor of Science (Biomedical Sciences)
Universidade Católica de Petrópolis, 2015
Candidate: Rafael Nicolay Batista da Silva.
Dissertation: Identificação de Enzimas Atuantes na Degradação de Celulose Utilizando Ferramentas de Bioinformática em Larga Escala.1
Jury: Afonso, A.O., Silva, M.L., Gomes, D.E.B.

Approvals in Public Concours (www.in.gov.br/)

2020 - Universidade Federal do Rio de Janeiro (DOU Seção 3, nº 83, 05/05/2021, p. 80)
Instituto de Biofísica Carlos Chagas Filho – Assistant Professor: Computational Biology

2019 - Universidade Federal do Rio de Janeiro (DOU Seção 3, nº 233, 03/12/2019, p. 85)
Instituto de Biofísica Carlos Chagas Filho – Assistant Professor: Structural Biology

2018 - Universidade Federal de Juiz de Fora (DOU Seção 1, nº 242, 18/12/ 2018, p.192)
Instituto de Ciências da Computação – Visinting Professor: Computational Modeling.

2015 - Universidade Federal de Minas Gerais (DOU Seção 3, nº 14, 21/01/2016, p.70)
Faculdade de Farmácia – Assistant Professor: Pharmaceutical/Medicinal Chemistry

2014 - Fundação Oswaldo Cruz. (DOU Seção 3, nº 122, 30/06/2014, p. 284)

[1] Identification of Cellulose-Degrating Enzymes Using High-Throughput Bioinformatics Tools

Research Scientist SP1619: Structural Biology and Bioimaging / Rio de Janeiro-RJ.

2013 - Universidade Federal do Rio de Janeiro. (DOU Seção 1, nº 167, 29/08/2013, p.14)
Substitute Professor, 2 years, 20h/w, Xerém. Structural Biology and Drug Design.

2012 - Laboratório Nacional de Computação Científica. (DOU Seção 3, nº 212, 01/11/2012, p.22)
Technologist: Computational Molecular Biophysics.

2012 - Universidade Federal do Rio de Janeiro. (DOU Seção 1, nº 40, 20/02/2012, p.12)
Substitute Professor, 2 years, 20h/w, Xerém. Structural Biology and Drug Design.

Student Co-Supervisions

Doctorate (Biotechnology) – National Institute of Standards – INMETRO, Brazil

2017 Rafael Mesquita Stoque.
The role of ionic liquids on the structure and dynamics of lignocellulosic complexes by computational and experimental methods.

Master in Computational Sciences – Universidade Federal de Juiz de Fora, Brazil.

2021. Ruan Carvalho Medina
Machine learning methods to predict binding free energies in Host-Guest systems.

Master (Biotechnology) National Institute of Standards – INMETRO, Brazil

2018 Thiciana Santos da Fonseca.
Analysis of the Thermostability of Cellulases in Ionic Liquids

2017 Kendy Anny de Azevedo Werneck.
Design of Selective Ligands for Tripanossomatides Sterol-Methil Transferase by Computational Modeling.

2016 Raquel Gama Gomes Leite.
Estudo de Complexos das Cisteíno-Proteases Plasmodiais Falcipaína-2 e Falcipaína-3 para o Desenho de Fármacos Antimaláricos

Master (Biophysics)

2020 Mariana Simões Ferreira
Computational studies of vivipains from *Plasmodium vivax*

2013 Rafael Mesquita Stoque.
Fluorimetry and Molecular Modeling Study of Dengue Virus Capsid Protein Mutations L81N, I88N, L81N-I88N e L50S.

2011 Priscila da Silva Figueiredo Celestino.
Study of Small Ligand Interation and Plasmodial Cysteine Proteases Falcipain-2 and 3

Undergraduate

2020 – 2021 Caio Cedrola Rocha (Computer Science – Universidade Federal de Juiz de Fora)
Machine learning methods applied to drug discovery against SARS-CoV-2 Main Protease.

2013-2016 Marcela Guimarães. (Biotechnology - Universidade Federal do Rio de Janeiro)
Identification, characterization and molecular modeling of lignocellulosic-degrading enzymes

2013-2015 Thiciana Santos da Fonseca. (Chemistry – Universidade do Grande Rio)
Molecular Modeling of Cellulose Fiber Weakening by Ionic Liquids.

2013-2014 Kendy Anne de Azevedo Werneck. (Univ. Católica de Petrópolis/INMETRO)
"Identificação e análise de celulases no metagenoma de Achatina fulica. "

2007-2009 Priscila da Silva Figueiredo Celestino. (UFRJ)
"Modelagem Computacional de Complexos de Enzimas do P. falciparum"

Master II (6 months, co-supervision)

2017 Cédric Bouysset (Université de Strasbourg)
Automatic Rescoring of Docking Resultsby end-point free energy approaches

2011 Elodie Japaud. (Université Paris Diderot / ENS-Cachan)
Developpement d'Un Outil de Prediction d'Arrimage Proteine-Proteine

Young Talent (High School) – Petrobras Fellowship

2014-2016 Wiliam Silva (Technician in Biotechnology - Colégio Estadual Círculo Operário)
Analise Estrutural de cadeias de Celulose e seus Complexos com Celulases por Métodos de Computacional de Modelagem Molecular

Foreign Languages (Native in Portuguese)

Language	-	Listen	-	Speak	-	Read	-	Write
Spanish	-	High	-	High	-	High	-	Medium
English	-	High	-	High	-	High	-	High
French	-	Medium	-	Low	-	Medium	-	Low