Lucas A. **Machado**

Computational Biologist/AI researcher ·
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Bio

Computational biologist working at the intersection of AI, bioinformatics, and computational chemistry. Skilled in applying Machine Learning and Molecular Modeling to analyze biological data, develop predictive models, and both comprehend and design biologically active molecules.

Education

Ph.D in Computational Biology *Rio de Janeiro, Brazil*
FIOCRUZ *2020*

MSc in Computational biology *Rio de Janeiro, Brazil*
FIOCRUZ *2016*

BSc in Biomedical Sciences *Rio de Janeiro, Brazil*
University of Vassouras *2013*
- Awarded with honors

Skills

Research expertise	Statistical Modeling, Network science, Protein structure and dynamics, Drug discovery, Protein engineering
AI	Pathogenicity prediction, QSAR, Language Models, AI-driven drug discovery
Programming	Python, R, BASH
Molecular modeling	GROMACS, Modeller, Alphafold2, MAESTRO (Schrödinger), pyRosetta, pymol, VMD
Technologies and libraries	Tensorflow, Scikit-learn, Linux, Git, RDkit, Pandas, numpy
Languages	Fluent english, Fluent Spanish, Native Portuguese, Basic French

Key achievements

- Helped elucidate drug-resistance mechanisms of HIV-1 using molecular modeling methods
- Elucidated key differences in proteins from bacterial strains used in the BCG vaccine, explaining their behavior through modeling
- Built Machine learning models to screen natural compounds for antiviral activity
- Developed statistical models for predicting Hydrogen/Deuterium exchange in proteins
- Characterized immunogenic proteins from *Acinetobacter baumannii* that were later used as targets for monoclonal antibodies

Experience

National Institute of Women, Children and Adolescents Health Fernandes Figueira/Fiocruz *Rio de Janeiro, Brazil*
Postdoctoral researcher - Computational Biology/AI research *May. 2023 - Now*
- Implement *in silico* routines for exome analysis
- Benchmark AI models for pathogenicity prediction
- Develop and use computational tools to help diagnose rare diseases

Oswaldo Cruz Institute/Fiocruz *Rio de Janeiro, Brazil*
Postdoctoral researcher - Protein engineering *Nov. 2022 - Mar. 2023*
- Implement *in silico* routines for optimizing therapeutic peptides using Rosetta
- Develop Machine learning models for optimizing search in sequence space
- Investigate *in silico* methods for protein stability optimization

University of Buenos Aires *Buenos Aires, Argentina*

Postdoctoral researcher - Drug discovery *Nov. 2021 - Nov. 2022*

- Predict protein structures and prepare the targets from multi-resistant bacteria for structure-based virtual screenings

Oswaldo Cruz Institute/Fiocruz *Rio de Janeiro, Brazil*

Postdoctoral researcher - Drug discovery *Apr. 2020 - Nov. 2021*

- Implement Machine Learning-based drug discovery pipelines

Oswaldo Cruz Institute/Fiocruz *Rio de Janeiro, Brazil*

Ph.D candidate *Aug. 2016 - Apr. 2020*

- Perform molecular dynamics simulations to investigate drug resistance mechanisms
- Structure prediction of Protein-DNA complexes
- Perform virtual screenings using Machine Learning models

Scientific Computing Program - Fiocruz *Rio de Janeiro, Brazil*

MSc candidate *Jan. 2014 - Jul. 2016*

- Perform normal mode analysis and molecular dynamics simulations
- Build statistical models to predict hydrogen/deuterium exchange in proteins

Bio-manguinhos immunobiological technology institute *Rio de Janeiro, Brazil*

BSc researcher *Jul. 2012, Dez. 2013*

- Find immunogenic proteins in Acinetobacter baumannii through reverse vaccinology methods
- Carry out bacterial growth and protein extraction
- Perform mice immunization and ELISA studies to verify the immune response

Honors & Awards

2023	**Selected as one of the 42 global competitors,** Merck Innovation Cup 2023	*Darmstadt, Germany*
2019	**Best Poster,** The Annual Meeting of the Brazilian Biophysical Society	*Santos, Brazil*
2018	**Best Poster,** The X-meeting	*São Pedro, Brazil*
2018	**Honorable mention,** IX School on Molecular Modeling of Biological Systems	*Petrópolis, Brazil*
2017	**Best Poster,** The X-meeting	*São Pedro, Brazil*
2016	**Honorable Mention,** III French-Brazilian Symposium on Biosciences	*Rio de Janeiro, Brazil*
2016	**Honorable Mention,** VIII School on Molecular Modeling of Biological Systems	*Petrópolis, Brazil*
2013	**Award for Highest grades,** Graduation	*Vassouras, Brazil*

Publications

Machado, L. A., Krempser, E., and Guimarães, A. C. R.. **A machine learning-based virtual screening for natural compounds capable of inhibiting the HIV-1 integrase**. Frontiers in Drug Discovery *2022*

Vieira de Araujo, A. E., Conde, L. V., da Silva Junior, H. C., **Machado, L. A.**, Lara, F. A., Chapeaurouge, A., Pauer, H., Pires Hardoim, C. C., Martha Antunes, L. C., D'Alincourt Carvalho-Assef, A. P., and Moreno Senna, J. P. **Cross-reactivity and immunotherapeutic potential of BamA recombinant protein from *Acinetobacter baumannii***. Microbes and Infection *2021*

Zabala-Peñafiel, A., Dias-Lopes, G., Cysne-Finkelstein, L., Conceição-Silva, F., Miranda, L. de F. C., Fagundes, A., Schubach, A. de O., Fernandes Pimentel, M. I., Souza-Silva, F., **Machado, L. A.**, and Alves, C. R. **Serine proteases profiles of *Leishmania* (Viannia) *braziliensis* clinical isolates with distinct susceptibilities to antimony**. Scientific reports *2021*

Schwarz, M. G. A., Luzes, B. G. C., Correa, P. R., Silva-Gonçalves, A. J. da, **Machado, L. A.**, Guimarães, A. C. R., and Mendonça-Lima, L. ***M. bovis* BCG Moreau N-Terminal Loss Leads to a Less Stable Dodecin With Lower Flavin Binding Capacity**. Frontiers in Cellular and Infection Microbiology *2021*

Machado, L. A. and Guimarães, A. C. R. **Evidence for Disruption of Mg2+ Pair as a Resistance Mechanism Against HIV-1 Integrase Strand Transfer Inhibitors**. Frontiers in Molecular Biosciences *2020*

Machado, L. A., Gomes, M. F. da C., and Guimarães, A. C. R. **Raltegravir-Induced Adaptations of the HIV-1 Integrase: Analysis of Structure, Variability, and Mutation Co-occurrence**. Frontiers in Microbiology *2019*