1. SUPPLEMENTARY MATERIAL - CURRENT MEMBERS AND RESEARCH PROJECTS

MEET THE MEMBERS

Raquel C. M. Minardi

Lab coordinator

Prof. Minardi has a Ph.D. in Bioinformatics from the Federal University of Minas Gerais and graduated in Computer Science at the same university. She also has a post-doctorate at Comissariat à lEnergie Atomique et aux Énergies Alternatives / CEA in France.
She is currently a Class D level 02 Professor in the Department of Computer Science at the Federal University of Minas Gerais (UFMG) and works as a permanent professor for the graduate programs in Computer Science and in Bioinformatics (both ranked as CAPES level 7).
She is an affiliate member of the Brazilian Academy of Sciences (2019-2023), Deputy coordinator of the Post-Graduation Program in Bioinformatics at UFMG (management 2020-2021 and 2022-2024).

Postdoctoral researcher

PhD in bioinformatics, master in bioinformatics, a post-doctoral internship at the Department of Computer Science at UFMG, focusing on the development of Web systems for Bioinformatics, exploratory analysis and data visualization. He has knowledge in languages: PHP, JavaScript, Python, R, Perl, HTML, CSS and SQL.

Diego Mariano
Ph.D. in Bioinformatics

Frederico C. Carvalho
Ph.D. student in Computer Science

Machine learning algorithms applied to computational structural biology problems

Peptide engineering is a field that still relies primarily on in vitro experiments, in a process of trial and error, to achieve its goals. We propose a computational pipeline that combines mechanistic models, machine learning and bioinspired algorithms to generate peptides optimized for functions of medical interest, bringing more efficiency, speed and precision to the area.

A database for the natural design of insecticides in natural products

The construction of a database of binders from natural products to be used in the rational design of new insecticides and fungicides, given their importance for the agribusiness sector.

Marcos José A. Viana
Ph.D. student in Bioinformatics

Luana Luisa Bastos
Ph.D. student in Bioinformatics

Protein-Protein Interaction Prediction through Structural Signatures and Machine Learning

The main objective is to develop a computational methodology based on structural signatures and machine learning for predicting the interaction of protein-protein complexes. Apply and evaluate the methodology to predict the interaction of tick proteins in the genus ixodes with proteins involved in the immune cascade such as TNF-alpha and interleukin 2.

Algorithms for rational design and optimization of peptidomimetic compounds for inhibition of potential SARS-CoV-2 targets

The project aims to use computational biology tools to develop a therapeutic strategy based on the design of new peptides that inhibit the Spike/ACE2 interaction.

Ana Paula de Abreu
Ph.D. student in Bioinformatics

Study of the action of aprotinin in the inhibition of SARS-CoV-2 and its impact on computational screening of molecules

The focus of the project is the inhibition of the TMPRSS2 protease, important for SARS-CoV-2 replication. We will mainly study aprotinin. The objective is to use machine learning and protein structure data to prospect molecules with potential action against the virus. As specific objectives, there is also the structural modeling of TMPRSS2, and the study of the action of aprotinin in this inhibition.

Vivian M. Paixão:
Masters' student in Bioinformatics

Models and algorithms for predicting the impact of mutations in the SARS-CoV-2 spike protein

Since Covid-19 has become one of the most worrisome diseases in recent times, mainly due to its characteristic of generating new variants, it becomes important to understand the best ways to fight it. For this, the development of methods capable of predicting the potential of mutations in the spike target protein can be of great importance to contain the disease in the world.

Eduardo U. M. Moreira
Masters' student in Bioinformatics

Machine learning models in the search for causes of autism

The increased incidence of autism may be related to substances present in everyday life, and that this occurs due to epigenetic modifications. The aim is to study this hypothesis by prospecting autism-causing molecules through machine learning. Structural virtual screening will be carried out for the selection of substances and analysis of candidate interactions with possible targets.

Alessandra G. Cioletti
Masters' student in Bioinformatics

Identification of conformational changes in proteins through distance maps and deep neural networks

The objective is to find out if convolutional neural networks are able to identify subtle conformational changes, caused by mutations in specific regions of proteins, from patterns found in distance maps. As a case study, we analyzed the spike protein receptor binding domain of SARS-CoV-2 as well as WHO-monitored mutations existing in this region.

Lucas M. dos Santos
Masters' student in Bioinformatics

Angie L. A. Puelles
Masters' student in Bioinformatics

Virtual Multi-Target Screening and Search for Pharmacophoric Signatures of Promising Phytochemical Compounds in the Treatment of Autism Spectrum Disorder

A promising pharmacological strategy in the treatment of Autism Spectrum Disorder is phytopharmaceutical therapy based on compounds of plant origin, as a curative benefit and reduction of side effects to conventional treatment. A number of phytochemical compounds have been shown to be capable of modulating the behavioral pattern in humans and promising new therapies and new drugs.

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Selene Melo
Undergraduate student in Information Systems

Gabriel D. de Oliveira
Undergraduate student in Control and Automation Engineering

E-Volve: understanding the impact of mutations in SARS-CoV-2 variants spike protein on antibodies and ACE2 affinity through patterns of chemical interactions at protein interfaces

Evolve is a Webtool designed to model mutations in the input protein complex using Modeller. Then, uses VTR to calculate and compare the protein contacts. In this project, our aim was to create an algorithm (E-volve) to analyze the impact of SARS-CoV-2 Spike protein mutations on the interaction with the ACE2 receptor and antibodies.

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Giovana de C. F. Maia
Undergraduate student in Biological Sciences