Supplementary material of "Bioinformatics and Computational Biology Research at the Department of Computer Science at UFMG"

Summary

Supplementary Table S1. Concluded and ongoing students.

Name	Level	Status	Year	Scholarship
Caio Júlio Martins Veloso	Ph.D.	Concluded	2007	No
Carlos Henrique da Silveira	Ph.D.	Concluded	2008	No
Raquel Cardoso de Melo Minardi	Ph.D.	Concluded	2008	Yes
Cristina Ribeiro	Ph.D.	Concluded	2009	Yes
Valdete Maria Gonçalves de Almeida	Ph.D.	Concluded	2011	Yes
Deive Ciro de Oliveira	Ph.D.	Concluded	2011	Yes
Douglas Eduardo Valente Pires	Ph.D.	Concluded	2012	Yes
Sabrina de Azevedo Silveira	Ph.D.	Concluded	2013	Yes
Felipe Ferré	Ph.D.	Concluded	2013	Yes
Wellisson Rodrigo dos Santos	Master	Concluded	2015	No
Alexandre Victor Fassio	Master	Concluded	2015	Yes
Pedro Magalhães Martins	Master	Concluded	2015	Yes
Nilma Rodrigues Alves	Ph.D.	Concluded	2015	No
Elisa Boari de Lima	Ph.D.	Concluded	2015	Yes
João Arthur Ferreira Gadelha Campelo	Ph.D.	Concluded	2017	No
José Renato de Moura Silva Barroso	Master	Concluded	2017	Yes
Laerte Mateus Rodrigues	Ph.D.	Concluded	2017	Yes
Francisco de Assis Sobrinho	Master	Concluded	2018	Yes
Diego César Batista Mariano	Ph.D.	Concluded	2019	Yes
Biharck Muniz Araújo	Ph.D.	Concluded	2019	No
Wandré Nunes Pinho Veloso	Ph.D.	Concluded	2019	No
Naiara de Almeida Pantuza	Master	Concluded	2019	Yes
Alexandre Victor Fassio	Ph.D.	Concluded	2019	Yes
Pedro Magalhães Martins	Ph.D.	Concluded	2020	Yes
Letícia Xavier Quintão	Master	Concluded	2021	Yes
Charles Abreu Santana	Pd.D.	Concluded	2021	Yes
Luana Luiza Bastos	Master	Concluded	2021	Yes
Lucas Moraes dos Santos	Master	Ongoing	-	No
Eduardo Utsch Madureira Moreira	Master	Ongoing	-	Yes
Vivian Morais Paixão	Master	Ongoing	-	Yes
Marcos José Andrade Viana	Ph.D.	Ongoing	-	No
Luana Luiza Bastos	Ph.D.	Ongoing	-	Yes
Frederico Chaves Carvalho	Ph.D.	Ongoing	-	Yes
Angie Lissette Atoche Puelles	Master	Ongoing	-	Yes
Alessandra Martins Cioletti	Master	Ongoing	-	No
Eduardo José Azevedo Correa	Ph.D.	Ongoing	-	No
Ana Paula Abreu	Ph.D.	Ongoing	-	Yes
Giovana de Castro Fiorini Maia	Undergraduate	Ongoing	-	Yes

Gabriel Dutra de Oliveira	Undergraduate	Ongoing	-	Yes
Selene Melo	Undergraduate	Ongoing	-	No

Supplementary Table S2. IDs and citations of group publications from 2003-2022.

ID	Paper
A1	DOS-SANTOS, VP et al.. 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. PeerJ, v. 10, p. e13099, 2022.
A2	MARTINS, P. M. et al.. Propedia: a database for protein-peptide identification based on a hybrid clustering algorithm. BMC BIOINFORMATICS, v. 22, p. 1-20, 2021.
A3	DOS-SANTOS, VP et al.. VTR: A Web Tool for Identifying Analogous Contacts on Protein Structures and Their Complexes. Frontiers in Bioinformatics, v. 1, p. 28, 2021.
A4	SILVA, A. L. et al.. From in-person to the online world: insights into organizing events in Bioinformatics. Frontiers in Bioinformatics, v. 1, p. 1-1, 2021.
A5	MELO-MINARDI, R. C.; BASTOS, L. L.. Expandindo as paredes da sala de aula aprendizados com o ensino a distância e ensino remoto emergencial. Revista da Universidade Federal de Minas Gerais, v. 28, p. 105-125, 2021.
A6	RIBEIRO, VAGNER S. et al.. visGReMLIN: graph mining-based detection and visualization of conserved motifs at 3D protein-ligand interface at the atomic level. BMC BIOINFORMATICS, v. 21, p. 80-92, 2020.
A7	MARIANO, D. et al.. Glutantbetaase: a database for improving the rational design of glucose-tolerant beta-glucosidases. BMC Molecular and Cell Biology, v. 21, p. 1-15, 2020.
A8	LIMA, LHF; et al.. Conformational flexibility correlates with glucose tolerance for point mutations in beta-glucosidases - A computational study. JOURNAL OF BIOMOLECULAR STRUCTURE \& DYNAMICS, v. 1, p. 1-20, 2020.
A9	BARROSO, JR et al.. Proteus: An algorithm for proposing stabilizing mutation pairs based on interactions observed in known protein 3D structures. BMC BIOINFORMATICS, v. 21, p. 275, 2020.
A10	SANTANA, CHARLES A. et al.. GRaSP: a graph-based residue neighborhood strategy to predict binding sites. BIOINFORMATICS, v. 36, p. i726-i734, 2020.
A11	SILVA, MARCOS F.M. et al.. Proteingo: Motivation, user experience, and learning of molecular interactions in biological complexes. ENTERTAINMENT COMPUTING, v. 29, p. 31-42, 2019.
A12	MARIANO, D. et al.. A Computational Method to Propose Mutations in Enzymes Based on Structural Signature Variation (SSV). INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES, v. 20, p. 333, 2019.
A13	MARIANO, D. et al.. Introducing Programming Skills for Life Science Students. BIOCHEMISTRY AND MOLECULAR BIOLOGY EDUCATION, v. 47, p. 1-8, 2019.
A14	COSTA, LSC et al.. Molecular Dynamics Gives New Insights into the Glucose Tolerance and Inhibition Mechanisms on beta-Glucosidases. MOLECULES, v. 24, p. 3215, 2019.
A15	FASSIO, A. et al.. nAPOLI: a graph-based strategy to detect and visualize conserved protein-ligand interactions in large-scale. IEEE-ACM Transactions on Computational Biology and Bioinformatics, p. 1-1, 2019.
A16	SOARDI, FERNANDA C. et al.. Familial STAG2 germline mutation defines a new human cohesinopathy. npj Genomic Medicine, v. 2, p. 1-11, 2017.
A17	MARIANO, D.C.B. et al.. Characterization of glucose-tolerant beta-glucosidases used in biofuel production under the bioinformatics perspective: a systematic review. GENETICS AND MOLECULAR RESEARCH, v. 16, p. gmr16039740, 2017.
A18	FASSIO, ALEXANDRE V. et al.. Vermont: a multi-perspective visual interactive platform for mutational analysis. BMC BIOINFORMATICS, v. 18, p. 51-79, 2017.
A19	BOARI-LIMA, ELISA; Meira, Wagner; MELO-MINARDI, RAQUEL CARDOSO DE . Isofunctional Protein Subfamily Detection Using Data Integration and Spectral Clustering. PLOS COMPUTATIONAL BIOLOGY (ONLINE), v. 12, p. e1005001, 2016.
A20	GONALVES, W. R. S. et al.. PDBest: a user-friendly platform for manipulating and enhancing protein structures. Bioinformatics (Oxford. Print), v. 31, p. btv223, 2015.

A21	AZEVEDO-SILVEIRA, S. A. et al.. ENZYMAP: Exploiting Protein Annotation for Modeling and Predicting EC Number Changes in UniProt/Swiss-Prot. Plos One, v. 9, p. e89162, 2014.
A22	AZEVEDO-SILVEIRA, SABRINA; et al.. VERMONT: Visualizing mutations and their effects on protein physicochemical and topological property conservation. BMC Proceedings, v. 8, p. S4, 2014.
A23	IZIDORO, S. C.; MELO-MINARDI, R. C.; PAPPA, G. L. . GASS: Identifying Enzyme Active Sites with Genetic Algorithms. BIOINFORMATICS, v. 1, p. 1, 2014.
A24	PIRES, D. et al.. aCSM: noise-free graph-based signatures to large-scale receptor-based ligand prediction. Bioinformatics (Oxford. Print), v. 29, p. 855-861, 2013.
A25	Bastard, K et al.. Revealing the hidden functional diversity of an enzyme family. Nature Chemical Biology, v. 10, p. 42-49, 2013.
A26	GONÇALVES-ALMEIDA, V. M. et al.. HydroPaCe: understanding and predicting cross-inhibition in serine proteases through hydrophobic patch centroids. Bioinformatics (Oxford. Print), v. 28, p. 342-349, 2012.
A27	PIRES, D. E. V. et al.. FPCluster: An Efficient Out-of-core Clustering Strategy without a Similarity Metric. Journal of Information and Data Management - JIDM, v. 3, p. 132, 2012.
A28	Arumugam, Manimozhiyan Raes, et al.. Enterotypes of the human gut microbiome. Nature (London), p. 1-7, 2011.
A29	Pires, Douglas et al.. Cutoff Scanning Matrix (CSM): structural classification and function prediction by protein inter-residue distance patterns. BMC GENOMICS, v. 12, p. S12, 2011.
A30	Bellinzoni, M. et al.. 3-keto-5-aminohexanoate cleavage enzyme: a common fold for an uncommon Claisen-type condensation. The Journal of Biological Chemistry (Print), v. 286, p. 27399-27405, 2011.
A31	Qin, Junjie Li et al.. A human gut microbial gene catalogue established by metagenomic sequencing. Nature (London), v. 464, p. 59-65, 2010.
A32	Ribeiro, Cristina et al.. Analysis of binding properties and specificity through identification of the interface forming residues (IFR) for serine proteases in silico docked to different inhibitors. BMC Structural Biology (Online), v. 10, p. 36, 2010.
A33	MELO-MINARDI, R. C.; BASTARD, K.; ARTIGUENAVE, F. . Identification of subfamily-specific sites based on active sites modeling and clustering. Bioinformatics (Oxford. Print), v. 26, p. 3075-3082, 2010.
A34	EHRLICH, D Antolin et al.. Metagenomics of the intestinal microbiota: potential applications. Gastroentérologie Clinique et Biologique, v. 34, p. S23-S28, 2010.
A35	da Silveira, Carlos H. et al.. Protein cutoff scanning: A comparative analysis of cutoff dependent and cutoff free methods for prospecting contacts in proteins. Proteins (Print), v. 74, p. 727-743, 2009.
A36	Gomide, J. et al.. Using linear algebra for protein structural comparison and classification. Genetics and Molecular Biology (Impresso), v. 32, p. 645-651, 2009.
A37	MELO-MINARDI, R. C. et al.. Finding protein-protein interaction patterns by contact map matching. Genetics and Molecular Research, v. 6, p. 1-10, 2007.
A38	VELOSO, C. J. M. et al.. On the characterization of energy networks of proteins. Genetics and Molecular Research, v. 6, p. 799-820, 2007.
A39	MELO-MINARDI, R. C. et al.. A contact map matching approach to protein structure similarity analysis. Genetics and Molecular Research, v. 5, p. 284-308, 2006.
A40	NESHICH, G. et al.. Star STING server: a multiplatform environment for protein structure analysis. Genetics and Molecular Research, v. 5, p. 717-722, 2006.
A41	PRADO, T. A. K. L. et al.. Using structural signatures for identifying globins: the intrasubunit electrostatics interactions. Revista Tecnologia da Informação, v. 3, p. 115-118, 2003.

Supplementary text 1. Current members and research projects

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