CURRICULUM VITAE

PERSONAL INFORMATION

Name: Dinler Amaral Antunes

Present Rank: Postdoctoral Research Associate

Date of Birth: August 11th, 1985

Sex: Male

Citizenship: Brazilian

Marital Status: Single

Webpage: http://goo.gl/3REiVp

Curriculum Lattes (Brazil):
http://lattes.cnpq.br/5578389590620746

PRIORITY FIELDS OF INTEREST

Dinler Antunes is a Postdoctoral Research Associate at the Computer Science Department of Rice University (Houston, TX), interested in structural bioinformatics and immunology. He is working with structural prediction of peptide-MHC (pMHC) complexes, with applications to cell-based immunotherapy against cancer. He is developing new docking-based methods to predict binding modes of large peptides to MHC-I receptors, aiming to explore MHC allotypes with special biomedical interest.

He attained his BS degree in Biomedicine in 2008, at the Federal University of Rio Grande do Sul (UFRGS, Brazil), and received a MS in Genetics and Molecular Biology from the same University in 2011. During his PhD, concluded in 2014, he applied bioinformatics tools to identify molecular features responsible for complex immunological phenomena, such as heterologous immunity. His work has shown *in silico* predictions of T cell cross-reactivity among viral epitopes, which were later confirmed by *in vitro* experiments. He is also a monthly contributor of the Brazilian Society of Immunology Blog (SBlogI).

Key words: immunology, immunotherapy, cross-reactivity, MHC, HLA and molecular docking.

FORMAL EDUCATION

BSc	Federal University of Rio Grande do Sul (UFRGS) – RS/Brazil	2005 – 2008
MSc	Federal University of Rio Grande do Sul (UFRGS) – RS/Brazil	2009 – 2011
PhD	Federal University of Rio Grande do Sul (UFRGS) – RS/Brazil	2011 – 2014
Postdoc	Rice University – Texas, USA	2014 – 2015
Postdoc	Rice University – Texas, USA	2015 – to date

AWARDS & FELLOWSHIPS

Best poster award in structural biology, 22nd Annual Sealy Center for Structural Biology & Molecular Biophysics Symposium	2017
Best poster presentation in the Development of Novel Therapies Through Fragment Based Drug Discovery (FBDD) meeting, for the work *Incremental Docking of Overlapping Fragments for Structural Prediction of Peptide-MHC complexes*.	2016
Postdoctoral fellowship through the Brazilian Scientific Mobility Program (*Ciências sem Fronteiras*, CNPq)	2014
Research travel award for short mission abroad. Conceded by the Federal University of Rio Grande do Sul (UFRGS, Brazil) to stablish a new collaboration with a research group at the Hannover Medical School (Hannover, Germany).	2012
Best poster presentation at the Biomedicine and Immunoinformatics session of the International Society for Computational Biology (ISCB) meeting, for the work *Hierarchical Clustering of pMHC Complexes Based on the Electrostatic Potential of the TCR-Interacting Surface.*	2012
Ph.D fellowship, *Conselho Nacional de Desenvolvimento Científico e Tecnológico* (CNPq)	2011 – 2014
M.Sc fellowship, *Conselho Nacional de Desenvolvimento Científico e Tecnológico* (CNPq)	2009 – 2011
Best poster presentation in the session Molecular Genetics, at the XIX *Salão de Iniciação Científica* of the Federal University of Rio Grande do Sul (UFRGS, Brazil).	2009
Scientific Initiation fellowship, *Conselho Nacional de Desenvolvimento Científico e Tecnológico* (PIBIC CNPq/UFRGS)	2006 – 2008

OTHER EXPERIENCE AND PROFESSIONAL MEMBERSHIPS

Permanent contributor of the Brazilian Society for Immunology Blog (SBlogI), Brazilian Society for Immunology (SBI)	2014 – to date
Student representative member of the research committee (COMPESQ), Institute for Health Basic Sciences of the Federal University of Rio Grande do Sul (ICBS-UFRGS)	2006 – 2008

INVOLVEMENT IN FUNDED RESEARCH PROJECTS

Structural modeling of peptide-HLA complexes presenting a melanoma-associated antigen for cross-reactivity assessment. Project supported by the Cancer Prevention & Research Institute of Texas (CPRIT, grant number RP170508). Participation as a co-author of the proposal and key personnel for the execution of the project.	2016
Structure-based Selection of Tumor-antigens for T-cell Based Immunotherapy. Project supported by NIH (R21, grant number 1R21CA209941-01), through the National Cancer Institute (NCI). Participation as a co-author of the proposal and key personnel for the execution of the project.	2016
Large-Scale MHC Epitope Analysis for Vaccine Development. Project supported by the Bill and Melinda Gates Foundation, through the Grand Challenges Explorations - Round 2. Participation as a co-author of the proposal and key personnel for the execution of the project.	2009

SCHOLARLY ACTIVITIES

Translation	
Human Molecular Genetics, 4th Edition (Tom Strachan / Andrew Read) - Chapter 1. Nucleic Acid Structure and Gene Expression.	2013
Human Molecular Genetics, 4th Edition (Tom Strachan / Andrew Read) - Chapter 10. Model Organisms, Comparative Genomics, and Evolution.	2013
Human Molecular Genetics, 4th Edition (Tom Strachan / Andrew Read) - Chapter 13. Human Genetic Variability and Its Consequences.	2013
Human Molecular Genetics, 4th Edition (Tom Strachan / Andrew Read) – Glossary and Index.	2013

Review (*Referee*)	
Journal of Molecular Graphics and Modelling	2017 – to date
Committee Member for the Master's Thesis defense of Marcelo Alves de Souza Bragatte, titled "*Evaluation of kinship: screening viral targets through the structural comparison of flavivirus t-cell epitopes - the Zika virus model*". (Master's Degree in Genetics and Molecular Biology)	2017
Current Computer-Aided Drug Design	2016 – to date

IEEE/ACM Transactions on Computational Biology and Bioinformatics	2015 – to date
Computers in Biology and Medicine	2014 – to date
African Journal of Microbiology Research	2012
Participation as reviewer of the work of Julia Medeiros Sorrentino, titled "*Aromatase inhibition by Valproic Acid on Autism*". (Degree in Pharmacy)	2013
Participation as reviewer of the work of Pedro Magno Mentges, titled "*Docking of thrombin planned inhibitors derived from glycyrrhetic acid*". (Degree in Pharmacy)	2011

PARTICIPATION IN THE DEVELOPMENT OF TOOLS AND DATABASES

Dinler Antunes has experience with Linux OS, working mainly with shell-based scripting and having basic knowledge of Python, R, C and Perl. He has experience with the use of sequence-based immunoinformatics tools, mainly with predictors of the endogenous peptide presentation pathway (MHC-I pathway), and with structural bioinformatics tools for molecular modeling (Modeller), molecular docking (Autodock 4 and Autodock Vina) and Molecular Dynamics (Gromacs Package).

He was involved in the development of the following tools and databases:

- DINC (http://dinc.kavrakilab.org/): an incremental meta-docking approach for docking large ligands.
- DockTope (https://dirac.cesup.ufrgs.br): an automated docking-based method for structural prediction of pMHC complexes.
- CrossTope (http://www.crosstope.com.br/): a curate repository of pMHC structures, focused on immunogenicity and cross-reactivity.

PUBLICATIONS

Dinler Antunes has published 13 peer-reviewed papers, being six as the first author. He has also published 3 book chapters and one paper at the International Conference on Bioinformatics and Computational Biology (BIOCOMP'10, Las Vegas).

Manuscripts submitted for publication

1. **Antunes DA**, Moll M, Devaurs D, Jackson K, Lizée G, Kavraki LE. ***DINC webserver: protein-peptide docking using an incremental approach***. Manuscript accepted for publication in a special feature of Cancer Research.

2. **Antunes DA**, Devaurs D, Moll M, Lizée G, Kavraki LE. ***General prediction of peptide-MHC binding modes using incremental docking: A proof of concept***. Manuscript submitted to Scientific Reports.

Peer-reviewed published papers

1. Devaurs D, **Antunes DA**, Papanastasiou M, Moll M, Ricklin D, Lambris JD, Kavraki LE. *Coarse-grained conformational sampling of protein structure improves the fit to experimental hydrogen-exchange data*. Frontiers in Molecular Biosciences. 2017 Mar 10;4:13. PMID: 28344973.

2. **Antunes DA**, Devaurs D, Kavraki LE. *Understanding the challenges of protein flexibility in drug design*. Expert opinion on drug discovery, pages 1–13, sep 2015. ISSN 1746-045X. PMID: 26414598.

3. **Antunes DA**, Mendes MFA, Rigo MM, Sinigaglia M, Vieira, GF. *Improved structural method for T-cell cross-reactivity prediction*. Molecular Immunology. 2015 Oct;67(2 Pt B):303-10. PMID: 26141239.

4. Zhang S, Bakshi RK, Suneetha PV, Fytili P, **Antunes DA**, Vieira GF, Jacobs R, Klade CS, Manns MP, Kraft AR, Wedemeyer H, Schlaphoff V, Cornberg M. *Frequency, private specificity and cross-reactivity of pre-existing HCV-specific CD8+ T cells in HCV seronegative individuals: implication for vaccine responses.* Journal of Virology. 2015 Aug;89(16):8304-17. PMID: 26041301.

5. **Antunes DA**, Figueiredo DF, Rigo MM., Mendes MFA, Silva JP, Mayer FQ, Matte U, Giugliani R, Vieira GF, Sinigaglia M. *Lessons From Molecular Modeling Human A-L-Iduronidase*. Journal Of Molecular Graphics & Modelling, V. 54, P. 107-113, 2014. PMID: 25459762.

6. **Antunes DA**, Rigo MM, Sinigaglia M, De Medeiros RM, Junqueira, DM. Almeida, SEM, Vieira GF. *New Insights into the In Silico Prediction of HIV Protease Resistance to Nelfinavir*. Plos One, v. 9, p. e87520, 2014. PMID: 24498124.

7. Sinigaglia M, **Antunes DA**, Rigo MM, Chies JAB, Vieira GF. *CrossTope: a curate repository of 3D structures of immunogenic peptide: MHC complexes.* Database-Oxford, v.2013, p.bat002 - bat002, 2013. PMID: 23396301.

8. Rigo MM, **Antunes DA**, Sinigaglia M, Sinigaglia M, Cibulski SP, Chies JAB, Vieira GF. *Immunogenic epitopes of Hantaviruses' N protein are restricted to conserved regions.* Frontiers in Bioscience, v.17, p.1582, 2012. PMID: 22201821.

9. Campos FS, Dezen D, **Antunes DA**, Santos HF, Arantes TS, Cenci A, Gomes F, Lima FES, Brito WMED, Filho HCK, Batista HBCR, Spilki FR, Franco AC, Rijsewijk FAM, Roehe PM. *Efficacy of an inactivated, recombinant bovine herpesvirus type 5 (BoHV-5) vaccine.* Veterinary Microbiology, v.148, p.18 - 26, 2011. PMID: 20828945.

10. **Antunes DA**, Rigo MM, Silva JP, Cibulski SP, Sinigaglia M, Chies JAB, Vieira GF. *Structural in silico analysis of cross-genotype-reactivity among naturally occurring HCV NS3-1073-variants in the context of HLA-A*02:01 allele.* Molecular Immunology., v.48, p.1461 - 1467, 2011. PMID: 21513985.

11. Varela APM, Holz CL, Cibulski SP, Teixeira TF, **Antunes DA**, Franco AC, Roehe LR, Oliveira MT, Campos FS, Dezen D, Cenci A, Brito WMED, Roehe PM. *Neutralizing antibodies to bovine herpesvirus types 1 (BoHV-1) and 5 (BoHV-5) and its subtypes.* Veterinary Microbiology (Amsterdam. Print). , v.142, p.254 - 260, 2010. PMID: 19926411.

12. **Antunes DA**, Vieira GF, Rigo MM, Cibulski SP, Sinigaglia M, Chies JAB. *Structural Allele-Specific Patterns Adopted by Epitopes in the MHC-I Cleft and Reconstruction of MHC:peptide Complexes to Cross-Reactivity Assessment.* Plos One, v.5, p.e10353, 2010. PMID: 20442757.

13. Rigo MM, **Antunes DA**, Vieira GF, Chies JAB. *MHC:Peptide Analysis: Implications on the Immunogenicity of Hantaviruses N protein.* Lecture Notes in Computer Science. , v.5676, p.160 - 163, 2009.

Complete work published in a congress

1. Fülber, C.C., **Antunes, D. A.**, Rigo, M. M., Chies, J. A. B., Sinigaglia, M., Vieira, G. F.
Reconstruction of MHC Alleles by Cross Modeling and Structural Assessment In: International Conference on Bioinformatics and Computational Biology, 2010, Las Vegas. **BIOCOMP'10, USA**., 2010.

Book Chapters

1. Rigo, M. M., **Antunes, D.A.**, Sinigaglia, M., Chies, J. A. B., Vieira, G. F.
MHC, Viral Infection and Immunoinformatics In: Major Histocompatibility Complex: Biology, Functions and Roles in Disease ed. Hauppauge : Nova Science Publishers, 2012

2. **Antunes, D.A.**, Rigo, M. M., Sinigaglia, M., Vieira, G. F.
Structural Immunoinformatics and Vaccine Development In: Bioinformatics Research: New Developments ed. Hauppauge : Nova Science Publishers, 2012

3. Rigo, M. M., **Antunes, D. A.**, Sinigaglia, M., Fülber, C.C., Chies, J. A. B., Vieira, G. F.
Molecular aspects involved in the immunogenicity against viral epitopes: an immunoinformatic perspective In: Immunogenicity ed. Hauppauge : Nova Science Publishers, 2010