

# DINLER A. ANTUNES, DSc

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## EDUCATION

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**Rice University, Houston, TX** Oct. 2014 – present  
Position: Postdoctoral Research Associate *Field of Study: Computational Biology and Cancer Immunotherapy*

**Federal University of Rio Grande do Sul (UFRGS), Porto Alegre, Brazil** Jun. 2011 – Aug. 2014  
Degree: DSc (Doctor of Science) *Field of Study: Bioinformatics and Viral Immunology*

**Federal University of Rio Grande do Sul (UFRGS), Porto Alegre, Brazil** Apr. 2009 – Mar. 2011  
Degree: MSc (Master of Science) *Field of Study: Genetics and Molecular Biology*

**Federal University of Rio Grande do Sul (UFRGS), Porto Alegre, Brazil** Mar. 2005 – Mar. 2009  
Degree: BSc (Bachelor of Science) *Field of Study: Biomedicine*

## AWARDS AND FELLOWSHIPS

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- 2019 Selected with honorable mention to the Rice U. School of Engineering's *Future Faculty Fellows Program*
- 2019 Fellowship from the *Computational Cancer Biology Training Program (CCBTP)*
- 2017 Best poster award at *22nd Annual Sealy Center for Structural Biology & Molecular Biophysics Symposium*
- 2016 Research travel award to attend to the *Immune Epitope Database (IEDB) Workshop* (San Diego, CA)
- 2016 Best poster award at *Development of Novel Therapies Through Fragment Based Drug Discovery Meeting*
- 2014–2015 Postdoctoral fellowship through the *Brazilian Scientific Mobility Program (Ciências sem Fronteiras/CNPq)*
- 2012 Research travel award to visit the Hannover Medical School (Hannover, Germany)
- 2012 Best poster award at *International Society for Computational Biology Latin American Regional Meeting*
- 2011–2014 DSc fellowship, *National Council for Scientific and Technological Development (CNPq)*
- 2009–2011 MSc fellowship, *National Council for Scientific and Technological Development (CNPq)*
- 2009 Best poster award at *XXI Salão de Iniciação Científica da UFRGS*; Poster presented by Cassiana Fülber
- 2007 Best poster award at *XIX Salão de Iniciação Científica da UFRGS*
- 2006–2008 Scientific Initiation fellowship, *National Council for Scientific and Technological Development (CNPq)*

## RESEARCH INTERESTS

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- Computational Biology
- Structural Bioinformatics
- Biomedical Informatics
- Cancer Immunotherapy
- Vaccine Development
- Drug Discovery

## PUBLICATIONS

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### Peer-Reviewed Journal Articles

23. **D. A. Antunes**, J. R. Abella, S. Hall-Swan, D. Devaurs, M. Moll, G. Lizée, and L. E. Kavraki. HLA-Arena: A customizable environment for the structural modeling and analysis of peptide-HLA complexes for cancer immunotherapy. (*Manuscript submitted for publication in JCO Clinical Cancer Informatics.*)
22. C. F. Soon, S. Zhang, P. V. Suneetha, **D. A. Antunes**, M. P. Manns, S. Raha, C. Schultze-Florey, I. Prinz, H. Wedemeyer, M. Sallberg Chen, and M. Cornberg. Hepatitis E Virus (HEV)-Specific T Cell Receptor Cross-Recognition: Implications for Immunotherapy. *Front. Immunol.*, 10:2076, 2019 ([pdf](#))

21. D. Devaurs, **D. A. Antunes**, S. Hall-Swan, N. Mitchell, M. Moll, G. Lizée, and L. E. Kavraki. Using parallelized incremental meta-docking can solve the conformational sampling issue when docking large ligands to proteins. *BMC Mol. Cell. Biol.*, 20(1):42, Sep 2019 ([pdf](#))
20. J. R. Abella, **D. A. Antunes**, C. Clementi, and L. E. Kavraki. APE-Gen: A fast method for generating ensembles of bound peptide-MHC conformations. *Molecules*, 24(5):881, Mar 2019 ([pdf](#))
19. **D. A. Antunes**, J. R. Abella, D. Devaurs, M. M. Rigo, and L. E. Kavraki. Structure-based methods for binding mode and binding affinity prediction for peptide-MHC complexes. *Curr. Top. Med. Chem.*, 18(26):2239–2255, 2018 ([pdf](#))
18. Didier Devaurs, **D. A. Antunes**, and Lydia E. Kavraki. Revealing unknown protein structures using computational conformational sampling guided by experimental hydrogen-exchange data. *Int. J. Mol. Sci.*, 19(11):3406, 2018 ([pdf](#))
17. **D. A. Antunes**, D. Devaurs, M. Moll, G. Lizée, and L. E. Kavraki. General Prediction of Peptide-MHC Binding Modes Using Incremental Docking: A Proof of Concept. *Sci. Rep.*, 8(1):4327, Mar 2018 ([pdf](#))
16. **D. A. Antunes**, M. M. Rigo, M. V. Freitas, M. F. A. Mendes, M. Sinigaglia, G. Lizée, L. E. Kavraki, L. K. Selin, M. Cornberg, and G. F. Vieira. Interpreting T-cell cross-reactivity through structure: Implications for TCR-based cancer immunotherapy. *Front. Immunol.*, 8:1210, 2017 ([pdf](#))
15. **D. A. Antunes**, M. Moll, D. Devaurs, K. R. Jackson, G. Lizée, and L. E. Kavraki. DINC 2.0: A New Protein-Peptide Docking Webserver Using an Incremental Approach. *Cancer Res.*, 77(21):e55–e57, Nov 2017 ([pdf](#))
14. D. Devaurs, **D. A. Antunes**, M. Papanastasiou, M. Moll, D. Ricklin, J. D. Lambris, and L. E. Kavraki. Coarse-Grained Conformational Sampling of Protein Structure Improves the Fit to Experimental Hydrogen-Exchange Data. *Front. Mol. Biosci.*, 4:13, 2017
13. Didier Devaurs, Malvina Papanastasiou, **D. A. Antunes**, Jayvee R. Abella, Mark Moll, Daniel Ricklin, John D. Lambris, and Lydia E. Kavraki. Native state of complement protein C3d analysed via hydrogen exchange and conformational sampling. *Int. J. Comput. Biol. Drug. Des.*, 11(1/2):90–113, 2016
12. M. F. Mendes\*, **D. A. Antunes\***, M. M. Rigo, M. Sinigaglia, and G. F. Vieira. Improved structural method for T-cell cross-reactivity prediction. *Mol. Immunol.*, 67(2 Pt B):303–310, Oct 2015. \* These authors contributed equally to this work
11. **D. A. Antunes**, D. Devaurs, and L. E. Kavraki. Understanding the challenges of protein flexibility in drug design. *Expert Opin. Drug. Discov.*, 10(12):1301–1313, Dec 2015
10. M. M. Rigo, **D. A. Antunes**, M. Vaz de Freitas, M. Fabiano de Almeida Mendes, L. Meira, M. Sinigaglia, and G. F. Vieira. DockTope: a Web-based tool for automated pMHC-I modelling. *Sci. Rep.*, 5:18413, Dec 2015
9. S. Zhang, R. K. Bakshi, P. V. Suneetha, P. Fytili, **D. A. Antunes**, G. F. Vieira, R. Jacobs, C. S. Klade, M. P. Manns, A. R. Kraft, H. Wedemeyer, V. Schlaphoff, and M. Cornberg. Frequency, private specificity, and cross-reactivity of preexisting hepatitis C virus (HCV)-specific CD8+ T cells in HCV-seronegative individuals: implications for vaccine responses. *J. Virol.*, 89(16):8304–8317, Aug 2015
8. D. F. Figueiredo\*, **D. A. Antunes\***, M. M. Rigo, M. F. Mendes, J. P. Silva, F. Q. Mayer, U. Matte, R. Giugliani, G. F. Vieira, and M. Sinigaglia. Lessons from molecular modeling human  $\alpha$ -L-iduronidase. *J. Mol. Graph. Model.*, 54:107–113, Nov 2014. \* These authors contributed equally to this work
7. **D. A. Antunes**, M. M. Rigo, M. Sinigaglia, R. M. de Medeiros, D. M. Junqueira, S. E. Almeida, and G. F. Vieira. New insights into the in silico prediction of HIV protease resistance to nelfinavir. *PLoS ONE*, 9(1):e87520, 2014
6. M. Sinigaglia, **D. A. Antunes**, M. M. Rigo, J. A. Chies, and G. F. Vieira. CrossTope: a curate repository of 3D structures of immunogenic peptide:MHC complexes. *Database (Oxford)*, 2013:bat002, 2013
5. M. M. Rigo, **D. A. Antunes**, S. P. Cibulski, M. Sinigaglia, J. A. Chies, and G. F. Vieira. Immunogenic epitopes of Hantaviruses' N protein are restricted to conserved regions. *Front. Biosci. (Landmark Ed)*, 17:1582–1588, Jan 2012

4. F. S. Campos, D. Dezen, **D. A. Antunes**, H. F. Santos, T. S. Arantes, A. Cenci, F. Gomes, F. E. Lima, W. M. Brito, H. C. Filho, H. B. Batista, F. R. Spilki, A. C. Franco, F. A. Rijsewijk, and P. M. Roehe. Efficacy of an inactivated, recombinant bovine herpesvirus type 5 (BoHV-5) vaccine. *Vet. Microbiol.*, 148(1):18–26, Feb 2011
3. A. P. Varela, C. L. Holz, S. P. Cibulski, T. F. Teixeira, **D. A. Antunes**, A. C. Franco, L. R. Roehe, M. T. Oliveira, F. S. Campos, D. Dezen, A. Cenci, W. D. Brito, and P. M. Roehe. Neutralizing antibodies to bovine herpesvirus types 1 (BoHV-1) and 5 (BoHV-5) and its subtypes. *Vet. Microbiol.*, 142(3-4):254–260, May 2010
2. **D. A. Antunes**, M. M. Rigo, J. P. Silva, S. P. Cibulski, M. Sinigaglia, J. A. Chies, and G. F. Vieira. Structural in silico analysis of cross-genotype-reactivity among naturally occurring HCV NS3-1073-variants in the context of HLA-A\*02:01 allele. *Mol. Immunol.*, 48(12-13):1461–1467, Jul 2011
1. **D. A. Antunes**, G. F. Vieira, M. M. Rigo, S. P. Cibulski, M. Sinigaglia, and J. A. Chies. Structural allele-specific patterns adopted by epitopes in the MHC-I cleft and reconstruction of MHC:peptide complexes to cross-reactivity assessment. *PLoS ONE*, 5(4):e10353, Apr 2010

### Peer-Reviewed Short-Articles/Extended Abstracts in Conference Proceedings

7. **D. A. Antunes**, D. F. Figueiredo, M. M. Rigo, J. P. Silva, J. A. Chies, M. Sinigaglia, and G. F. Vieira. Hierarchical clustering of pMHC complexes based on the electrostatic potential of the TCR-interacting surface. In *Second International Society for Computational Biology Latin American regional meeting (ISCB-Latin America)*, 2012. Santiago, Chile. (**best poster award**)
6. M. M. Rigo, **D. A. Antunes**, R. Minozzo, J. P. Silva, D. F. Figueiredo, J. A. Chies, M. Sinigaglia, and G. F. Vieira. Analysis of interaction residues between HLA-A\*02:01 cleft and epitopes. In *Second International Society for Computational Biology Latin American regional meeting (ISCB-Latin America)*, 2012. Santiago, Chile
5. C. C. Fülber, **D. A. Antunes**, M. M. Rigo, J. A. Chies, M. Sinigaglia, and G. F. Vieira. Reconstruction of MHC alleles by cross-modeling and structural assessment. In *International Conference on Bioinformatics and Computational Biology (BIOCOMP'10)*, pages 459–463, 2010. Las Vegas, NV
4. M. M. Rigo, **D. A. Antunes**, G. F. Vieira, and J. A. Chies. Immunogenic regions on the N protein from hantavirus genus: implications in vaccine development. In *Analys of the 4th International Conference of the Brazilian Association for Bioinformatics and Computational Biology (X-Meeting 2008)*, 2008. Salvador, Brazil
3. **D. A. Antunes**, G. F. Vieira, and J. A. Chies. Structural analyses of viral epitopes and proteolytic simulation of its proteins. In *Analys of 3rd International Conference of the Brazilian Association for Bioinformatics and Computational Biology (X-Meeting 2007)*, 2007. São Paulo, Brazil
2. G. F. Vieira, **D. A. Antunes**, and J. A. Chies. Viral epitopes: which is(are) the target(s)? In *Analys of 3rd International Conference of the Brazilian Association for Bioinformatics and Computational Biology (X-Meeting 2007)*, 2007. São Paulo, Brazil
1. M. M. Rigo, **D. A. Antunes**, G. F. Vieira, and J. A. Chies. MHC:Peptide analysis: Implications on the immunogenicity of hantaviruses' N protein. In *Advances in Bioinformatics and Computational Biology - BSB 2009*, Lecture Notes in Computer Science, pages 160–163. Springer, Berlin, Heidelberg, 2009. Porto Alegre, Brazil

### Book Chapters

3. **D. A. Antunes**, Rigo M. M., Sinigaglia M., and Vieira G. F. *Structural Immunoinformatics and Vaccine Development*, pages 1–33. Biotechnology in Agriculture, Industry and Medicine. Nova Science Publishers, 2012
2. Rigo M. M., **D. A. Antunes**, Sinigaglia M., Chies J. A. B., and Vieira GF. *MHC, Viral Infection and Immunoinformatics*, pages 69–85. Immunology and Immune System Disorders. Nova Science Publishers, 2012
1. M. M. Rigo, **D. A. Antunes**, M. Sinigaglia, C. C. Fülber, J. A. B. Chies, and G. F. Vieira. *Molecular aspects involved in the immunogenicity against viral epitopes: an immunoinformatic perspective*, pages 1–24. Immunology and Immune System Disorders. Nova Science Publishers, 2011

### Selected Poster Abstracts (out of a total of 58 posters presented in conferences)

- **D. A. Antunes**, D. Devaurs, M. Moll, G. A. Lizée, and L. E. Kavraki. Towards a general method for geometry prediction of peptide-HLA complexes: implications for immunotherapy. In *22nd Annual Structural Biology Symposium*, May 2017. Galveston, Texas. (**best poster award**)
- **D. A. Antunes**, M. Moll, K. Jackson, G. A. Lizée, and L. E. Kavraki. Incremental docking of overlapping fragments for structural prediction of peptide-MHC complexes. In *Development of Novel Therapies through Fragment Based Drug Discovery (FBDD)*, May 2016. Houston, Texas. (**best poster award**)
- C. C. Fülber, **D. A. Antunes**, M. M. Rigo, J. A. Chies, M. Sinigaglia, and G. F. Vieira. Reproduction of crystallographic structures of murine MHCs for the development of an approach for modeling unknown mhc structures. In *XXI Salão de Iniciação Científica da UFRGS*, October 2009. Porto Alegre, Brazil. (**best poster award**)
- **D. A. Antunes**, G. F. Vieira, and J. A. Chies. Computational simulation of proteasomal degradation of viral proteins, and structural analysis of immunodominant peptides. In *XIX Salão de Iniciação Científica da UFRGS*, October 2007. Porto Alegre, Brazil. (**best poster award**)

### Theses

3. **D. A. Antunes**. *Peptide:MHC structural similarity as a probability for cross-reactive T cell responses*. PhD thesis, Federal University of Rio Grande do Sul, Graduate Program in Genetics and Molecular Biology (PPGBM), August 2014. Language: Portuguese. ([pdf](#))
2. **D. A. Antunes**. *In silico study of the molecular basis for cross-reactivity between viral epitopes restricted to HLA-A\*02:01*. Master's thesis, Federal University of Rio Grande do Sul, Graduate Program in Genetics and Molecular Biology (PPGBM), March 2011. Language: Portuguese. ([pdf](#))
1. **D. A. Antunes**. *Use of bioinformatics tools for the analysis of cross-reactivity likelihood between viral epitopes*. Undergraduate thesis, Federal University of Rio Grande do Sul, Institute of Basic Health Sciences, August 2008. Language: Portuguese. ([pdf](#))

### **CONTRIBUTED SOFTWARE**

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**APE-Gen**: a fast method for generating ensembles of bound pMHC conformations.  
(<http://github.com/KavrakiLab/APE-Gen>)

**DINC**: a webserver for incremental meta-docking of large ligands.  
(<http://dinc.kavrakilab.org/>)

**DockTope**: a webserver for docking-based structural prediction of pMHC complexes.  
(<http://tools.iedb.org/docktope/>)

**CrossTope**: a curate repository of modeled pMHC structures, focused on immunogenicity and cross-reactivity.  
(<http://www.crosstope.com/>)

### **OTHER EXPERIENCE AND PROFESSIONAL MEMBERSHIPS**

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- Member of the International Society for Computational Biology (**ISCB**), 2019 – to date
- Coordinator of the Houston Chapter of an association of Brazilian researchers (**PUB Houston**), 2016 – to date
- Regular contributor to the Blog of the Brazilian Society for Immunology (**SBI**), 2014 – to date
- Student representative member of the research committee (**COMPESQ**) at the Institute for Basic Health Sciences of the Federal University of Rio Grande do Sul (**ICBS-UFRGS**), 2006 – 2008

## INVOLVEMENT IN FUNDED RESEARCH PROJECTS

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**Structural modeling and analysis of peptide-HLA complexes for cancer immunotherapy applications.** High-performance computing start up allocation through the Extreme Science and Engineering Discovery Environment ([XSEDE](#)). Project number MCB180187. **Role:** Principal Investigator (PI). **Allocation:** 1,600 SUs ( $\approx 4,961,504$  NUs).

**Structure-based Selection of Tumor-antigens for T-cell Based Immunotherapy.** Project supported by NIH, grant number [1R21CA209941-01](#), through the Informatics Technology for Cancer Research ([ITCR](#)) initiative of the National Cancer Institute (NCI). **Role:** Co-author of the proposal and key personnel for the execution of the project. **Total Funding:** US\$ 181,965.

**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](#). **Role:** Co-author of the proposal and key personnel for the execution of the project. **Total Funding:** US\$ 900,000.

**Large-Scale “MHC:Epitope” Analysis for Vaccine Development.** Project supported by the Bill and Melinda Gates Foundation, grant number [53049](#), through the Grand Challenges Explorations ([GCE](#))- Round 2. **Role:** Co-author of the proposal and key personnel for the execution of the project. **Total Funding:** US\$ 100,000.

## ADVISING OF STUDENTS

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### Advisor

Alexandra Bishop	summer undergrad. student	Rice University	2019
Thaís Cristine Arns	visiting student	Rice University	2016
Karen Wong	summer undergrad. student	Rice University	2015
Sujey Tadwalker	undergraduate student	Rice University	2015
Tahila Andrighetti	undergraduate student	UFRGS	2013
Jader P. da Silva	undergraduate student	UFRGS	2011 – 2012
Cassiana C. Fülber	undergraduate student	UFRGS	2009 – 2010
Bruna Correa	undergraduate student	UFRGS	2009

### Co-Advisor

Anja Conev	graduate student	Rice University	2019 – to date
Romanos Fasoulis	graduate student	Rice University	2019 – to date
Sarah Hall-Swan	graduate student	Rice University	2018 – to date
Kyle R. Jackson*	graduate student	UT MD Anderson	2016 – to date
Jayvee R. Abella*	graduate student	Rice University	2015 – to date
Marcus F. A. Mendes	graduate student	UFRGS	2012 – 2014
Martiel Freitas	undergraduate student	UFRGS	2013 – 2014
Renata F. Tarabini	undergraduate student	UFRGS	2013 – 2014
Caio Diniz	undergraduate student	UFRGS	2013
Francis Maria Bão Zambra	graduate student	UFRGS	2011 – 2012
Daniele F. Figueiredo	graduate student	UFRGS	2010 – 2012

\* Senior graduate students close to their PhD defense.

## ACADEMIC SERVICES

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### Committee Member for Thesis Defense

- Committee Member for the undergraduate Thesis of **Cristiane Trentin**, titled *3D homology modeling of the Acetylcholinesterase enzyme from Zebrafish*. Specialization in Computational Biology and Data Analysis. Universidade de Passo Fundo (UPF). Passo Fundo, Brazil. 2019.

- Committee Member for the undergraduate Thesis of **Cristian Guilherme Petry**, titled *Impact of energy minimization over residue-residue interactions and electrostatic potential on peptide-MHC-I complexes*. Specialization in Computational Biology and Data Analysis. Universidade de Passo Fundo (UPF). Passo Fundo, Brazil. 2019.
- Committee Member for the undergraduate Thesis of **Clarissa Taufer**, titled *Differentially expressed genes in melanoma for white and asian samples from TCGA that are not included in panels for clinical diagnostics*. Specialization in Computational Biology and Data Analysis. Universidade de Passo Fundo (UPF). Passo Fundo, Brazil. 2019.
- Committee Member for the undergraduate Thesis of **Edenilson Canabarro**, titled *Characterization of two complete genomes of Leptospira spp. isolated from outbreaks in dairy cattle*. Specialization in Computational Biology and Data Analysis. Universidade de Passo Fundo (UPF). Passo Fundo, Brazil. 2019.
- Committee Member for the Master's Thesis defense of **Matheus de Bastos Balb e Gutierres**, titled *Prediction of substrate binding to DNAK chaperone using machine learning*. Master's Degree in Molecular and Cell Biology. Pontifical Catholic University of Rio Grande do Sul (PUCRS). Porto Alegre, Brazil. 2019.
- Committee Member for the PhD Thesis defense of **Tha s Cristine Arns**, titled *Molecular modeling and dynamics of immunomodulatory molecule HLA-G*. Degree of Doctor of Science, with emphasis in Immunology. School of Medicine at Ribeir o Preto, University of S o Paulo (USP). Ribeir o Preto, Brazil. 2018.
- 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. Federal University of Rio Grande do Sul (UFRGS). Porto Alegre, Brazil. 2017.
- Committee Member for the undergraduate Thesis of **Julia Medeiros Sorrentino**, titled *Aromatase inhibition by Valproic Acid on Autism*. Bachelor Degree in Pharmacy. Federal University of Rio Grande do Sul (UFRGS). Porto Alegre, Brazil. 2013.
- Committee Member for the undergraduate Thesis of **Pedro Magno Mentges**, titled *Docking of thrombin planned inhibitors derived from glycyrrhetic acid*. Bachelor Degree in Pharmacy. Federal University of Rio Grande do Sul (UFRGS). Porto Alegre, Brazil. 2011.

### Committe Member for Conferences

- Program Committee Member for the *American Medical Informatics Association (AMIA) 2020 Informatics Summit*. Houston, TX. March 2020.
- Program Committee Member for the *First International Symposium on Mathematical and Computational Oncology (ISMCO'19)*. Lake Tahoe, NV. October 2019.

### Reviewer of Journal Articles

- *Bioinformatics*, Oxford Journals. 2019 – to date.
- *Journal of Chemical Information and Modeling*, American Chemical Society (ACS). 2019 – to date.
- *Cancer Immunology Research*, American Association for Cancer Research (AACR). 2018 – to date.
- *Current Topics in Medicinal Chemistry*, Bentham Science. 2018 – to date.
- *Computational Biology and Chemistry*, Elsevier. 2018 – to date.
- *Journal of Molecular Graphics and Modelling*, Elsevier. 2017 – to date.
- *Current Computer-Aided Drug Design*, Bentham Science. 2016 – to date.
- *IEEE/ACM Transactions on Computational Biology and Bioinformatics*. 2015 – to date.
- *Computers in Biology and Medicine*, Elsevier. 2014 – to date.
- *African Journal of Microbiology Research*, Academic Journals (AJ). 2012.

## Reviewer of Grants/Fellowships

- Ad-hoc expert reviewer on postdoctoral fellowship application for the *Auckland Medical Research Foundation* (New Zealand). 2018.

## Book Chapter Translations

- Tom Strachan and Andrew Read. *Human Molecular Genetics*, chapter Glossary and Index. Grupo A, 4th edition, 2013. ISBN: 9788565852517. Language: Portuguese. ([book intro](#))
- Tom Strachan and Andrew Read. *Human Molecular Genetics*, chapter 1. Nucleic Acid Structure and Gene Expression, pages 1–28. Grupo A, 4th edition, 2013. ISBN: 9788565852517. Language: Portuguese. ([pdf](#))
- Tom Strachan and Andrew Read. *Human Molecular Genetics*, chapter 10. Model Organisms, Comparative Genomics, and Evolution, pages 297–344. Grupo A, 4th edition, 2013. ISBN: 9788565852517. Language: Portuguese.
- Tom Strachan and Andrew Read. *Human Molecular Genetics*, chapter 13. Human Genetic Variability and Its Consequences, pages 405–440. Grupo A, 4th edition, 2013. ISBN: 9788565852517. Language: Portuguese.

## **LECTURES, TUTORIALS AND INVITED TALKS**

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### Lectures in classes for undergraduate and graduate students

- *Motion Planning for Large Molecular Complexes*. Lecture in the class “Algorithmic Robotics” (COMP 450), Prof. Lydia Kavradi. Graduate Program in Computer Science. Rice University. Houston, TX, US. 2019
- *Principal Component Analysis, K-means, and Clustering*. Lecture in the class “Biomedical Informatics” (COMP 573), Prof. Lydia Kavradi. Graduate Program in Computer Science. Rice University. Houston, TX, US. 2015
- *The role of the Biomedicine’s professional on academia (2nd Ed.)*. Lecture in the class “Cycle of lectures on Biomedicine’s professional paths” (BIM 99002), Prof. Denise M. Zancan. Bachelor’s course in Biomedicine, Federal University of Rio Grande do Sul. Porto Alegre, RS, Brazil. 2014
- *The role of the Biomedicine’s professional on academia*. Lecture in the class “Cycle of lectures on Biomedicine’s professional paths” (BIM 99002), Prof. Denise M. Zancan. Bachelor’s course in Biomedicine, Federal University of Rio Grande do Sul. Porto Alegre, RS, Brazil. 2013
- *Gene Therapy*. Lecture in the class “Genetics – Biotechnology” (BIO 07035), Prof. Lavinia Schüler-Faccini. Bachelor’s course in Biotechnology, Federal University of Rio Grande do Sul. Porto Alegre, RS, Brazil. 2012
- *Introduction to Proteomics and Structural Bioinformatics*. Lecture in the class “Genetics – Biotechnology” (BIO 07035), Prof. Lavinia Schüler-Faccini. Bachelor’s course in Biotechnology, Federal University of Rio Grande do Sul. Porto Alegre, RS, Brazil. 2012
- *Proteomics and Bioinformatics*. Experimental lecture in the class “Methods for teaching genetics to undergraduate students” (GEP 101), Prof. Claiton M. Ferreira. Graduate Program in Genetics and Molecular Biology, Federal University of Rio Grande do Sul. Porto Alegre, RS, Brazil. 2012
- *Bioinformatics: Origin and Applications*. Lecture in the class “Introduction to Science and Technology,” Prof. Cristiano Tolfo. Bachelor’s course in Computer Science, Universidade Federal do Pampa (UNIPAMPA). Alegrete, RS, Brazil. 2011
- *Bioinformatics: Origin and Applications*. Lecture in the class “Clinical Genetics,” Prof. Nance B. Nardi. Bachelor’s course in Medicine, Lutheran University of Brazil (ULBRA). Canoas, RS, Brazil. 2008

## Hands-on Tutorials/Workshops

- *Current methods and open challenges for structural modeling in cancer immunotherapy*. Tutorial held as part of the First International Symposium on Mathematical and Computational Oncology (ISMCO'19). Lake Tahoe, NV. Duration: 4 h. 2019
- *Bioinformatics (2nd Ed.)*. Tutorial held at the Methodist University Center (IPA). Porto Alegre, Brazil. Duration: 4 h. 2011
- *Bioinformatics*. Tutorial held at the Methodist University Center (IPA). Porto Alegre, Brazil. Duration: 4 h. 2010
- *Bioinformatics tools applied to vaccine development (2nd Ed.)*. Tutorial held at the Informatics Institute (INF) of the Federal university of Rio Grande do Sul (UFRGS). Porto Alegre, Brazil. Duration: 20 h. 2009
- *Bioinformatics tools applied to vaccine development*. Tutorial held at the Informatics Institute (INF) of the Federal university of Rio Grande do Sul (UFRGS). Porto Alegre, Brazil. Duration: 12 h. 2008
- *The role of bioinformatics on the development of new vaccination strategies*. Tutorial held at the Institute for Basic Health Sciences (ICBS) of the Federal university of Rio Grande do Sul (UFRGS). Porto Alegre, Brazil. Duration: 12 h. 2008
- *Bioinformatics tools applied to immunology*. Tutorial held at the Postgraduate Program in Genetics and Molecular Biology (PPGBM) of the Federal university of Rio Grande do Sul. Porto Alegre, Brazil. Duration: 20 h. 2007

## Invited Talks

- *Enabling structure-based data-driven selection of targets for cancer immunotherapy*. Talk scheduled for presentation at the Seventeenth Annual Rocky Mountain Bioinformatics Conference (Rocky19), a meeting of the International Society for Computational Biology (ISCB). Aspen/Snowmass, CO. Dec 5–7, 2019.
- *Large-scale modeling of class I peptide-HLA complexes using APE-Gen*. Talk at the First International Symposium on Mathematical and Computational Oncology (ISMCO'19). Lake Tahoe, NV. October 2019.
- *Applications of structural bioinformatics to cancer immunotherapy*. Talk at the XXII Semana Acadêmica da Biologia, Universidade de Passo Fundo (UPF). Passo Fundo, Brazil. September 2019.
- *Conformational sampling of large ligands made possible by a parallelized incremental meta-docking approach*. Talk at the annual meeting of the Informatics Technology for Cancer Research (ITCR). Salt Lake City, UT. May 2019.
- *Predicting binding modes of large peptides to MHC-I receptors*. Talk at the group meeting of Prof. Yousif Shamoo, Department of BioSciences, Rice University. Houston, TX. April 2018.
- *Structure-based selection of tumor-antigens for T-cell based immunotherapy*. Talk at the annual meeting of the Informatics Technology for Cancer Research (ITCR). Bethesda, MD. May 2018.
- *Towards personalized structural analysis of peptide-HLA complexes for T-cell-based immunotherapy*. Talk at the 2nd Genomic Medicine Conference (GeneMed-2018). Houston, TX. February 2018.
- *General structural prediction of peptide-HLA complexes*. Talk at the annual meeting of the Informatics Technology for Cancer Research (ITCR). Santa Cruz, CA. May 2017.
- *Structural bioinformatics applied to cancer*. Talk at the Seminar Series of the association of Brazilian researchers and academics (PUB Houston). Houston, TX. 2016
- *Customized docking method to perform binding mode prediction of large ligands to HLA molecules*. Talk at the meeting of the Postdoctoral Fellows of The Computational Cancer Biology Training Program (CCBTP). Houston, TX. 2015.
- *Peptide:MHC structural similarity as a probability for cross-reactive T cell responses*. Talk at the group meeting of Prof. John Lambris, Department of Pathology & Laboratory Medicine, University of Pennsylvania School of Medicine (Med.UPenn), Philadelphia. 2014.



- *Advances in Bioinformatics*. Talk at the Federal Institute for Education, Science and Technology Sul-Rio-Grandense (IFSul). Porto Alegre, RS, Brazil. 2014.
- *Application of bioinformatics to vaccinology*. Talk at the course on “Informatics applied to Biology and Drug Design,” Pontifical Catholic University of Rio Grande do Sul (PUCRS). Porto Alegre, RS, Brazil. 2011.
- *Biomedicine and Biotechnology: Paths to study different aspects of Biology*. Talk at a high school (Escola Estadual de Ensino Médio Demétrio Ribeiro). Alegrete, Brazil. 2011.
- *Bioinformatics for vaccine development*. Talk at the Lutheran University of Brazil (ULBRA). Canoas, Brazil. 2008.

## OTHER SKILLS

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**Languages:** *Portuguese* (mother tongue)                      *English* (fluent)                      *Spanish* (advanced)

**Computational skills:** Experience with shell-scripting (Linux), Perl and Python. Basic training on R and C. Experience with L<sup>A</sup>T<sub>E</sub>X, version control systems (Git, Mercurial, GitHub, GitLab), and containerization (Docker).

**Bioinformatics software:** Experience with the use of sequence-based immunoinformatics tools, and with structural bioinformatics tools for homology modeling, molecular docking, protein-protein docking, and molecular mechanics molecular dynamics (MMMD).

**Other certified training:** Grant Proposal Writing, Rigor and Reproducibility in Publication, Responsible Conduct of Research, Research Mentoring, Crafting Quality Code in Python, Financial Conflict of Interest.