DINLER A. ANTUNES, DSc

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PERSONAL STATEMENT

Dinler Antunes is a computational biologist interested in biomedical applications, including cancer immunotherapy, antiviral vaccine development, and drug discovery. He is developing computational methods to improve the safety and specificity of personalized cancer immunotherapy, and to facilitate structural analysis of intermolecular interactions.

EMPLOYMENT

University of Houston, Houston, TX Jan. 2021 – present
Position: Assistant Professor of Computational Biology *Department of Biology and Biochemistry*

Rice University, Houston, TX Oct. 2014 – Dec. 2020
Position: Postdoctoral Research Associate *Department of Computer Science*

EDUCATION

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

2020	Immuno-Oncology Young Investigators' Forum (IOYIF) PhD Postdoc Award (MD Anderson & SITC)
2020	SCI Gold Oral Presentation Award at the *6th Annual SCI Summer Research Colloquium* (Rice University)
2020	One of the 40 researchers selected for the Immuno-Oncology Young Investigators' Forum (IOYIF)
2019	Selected with honorable mention to the Rice U. School of Engineering's *Future Faculty Fellows Program*
2019–2020	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)

PUBLICATIONS

Since 2010, I have published 55 peer-reviewed articles in scientific journals, 27 of which (≃49%) have been published in the last 4 years, after I joined the University of Houston as an Assistant Professor. Since 2007, I have authored or co-authored over 100 poster abstracts (and oral presentations). From those, over half correspond to presentations made by trainees (mentored, co-mentored, collaborations) from after I joined the University of Houston in 2021. According to Google Scholar (see profile), I have a total of 1,807 citations, my h-index is 23, and my i10-index is 33.

Peer-Reviewed Journal Articles

Symbols used to highlight aspects of authorship and mentorship:
∗, shared first autorship.
∝, corresponding authorship.
‡, postdoctoral trainee working in my lab at UH.
†, graduate student trainee working in my lab at UH.
ψ, rotation graduate student working in my lab at UH.

55. F. Beruldsen[†], M. Vaz de Freitas[‡], and **D. A. Antunes**[∝]. High resolution mapping of protein motions in time and space with RMSX and Flipbook. *Scientific Reports*, 2026. manuscript accepted for publication

54. E. Dasdemir, I. Veletic, C. P. Ly, A. E. Quesada, C. D. Pacheco, F. Z. Jelloul, P. Borges[†], S. Basu, S. Jindal, Z. Wang, A. Lazar, K. M. Wani, **D. A. Antunes**, P. K. Reville, P. H. Gunaratne, R. J. Tower, P. Sharma, and H. Abbas[∝]. Integrative spatial multi-omics reveal niche-specific inflammatory signaling and differentiation hierarchies in acute myeloid leukemia. *iScience*, November 2025

53. F. J. F. de Sousa[†], **D. A. Antunes**[∝], and G. Zanatta[∝]. PI3K-Seeker: A Machine Learning-Powered Web Tool to Discover PI3K Inhibitors. *ACS Omega*, November 2025 (pdf).

52. M. B. Castillo, S. Rankothgedera, S. Thevasagayampillai, A. Kandasamy, J. Lewis[†], C. Woody, M. Vaz de Freitas[‡], **D. A. Antunes**, R. El-Zein, and P. H. Gunaratne[∝]. Identification of immunogenic KIF5B-RET fusion neopeptides driving immune stimulation in tumor specific CD8+ T cells. *Frontiers in immunology*, 16:1635810, 2025 (link).

51. P. Arman, Z. Haghighijoo, C. A. Lupascu, A. K. Singh, N. A. Goode, T. T. Baumgartner, J. Singh, Y. Xue, P. Wang, H. Chen, **D. A. Antunes**, M. Lijffijt, J. Zhou, M. Migliore, and F. Laezza[∝]. FGF14 Peptide Derivative Differentially Regulates Nav1.2 and Na(v)1.6 Function. *Life (Basel, Switzerland)*, 15(9), August 2025 (link).

50. C. C. Alves, J. Lewis[†], **D. A. Antunes**[∝], and E. A. Donadi[∝]. The role of vimentin peptide citrullination in the structure and dynamics of hla-drb1 rheumatoid arthritis risk-associated alleles. *Int J Mol Sci*, 34, January 2025 (link)

49. H. N. Le[†], M. Vaz de Freitas[‡], and **D. A. Antunes**[∝]. Strengths and limitations of web servers for the modeling of TCRpMHC complexes. *Comput Struct Biotechnol J*, 23, July 2024 (pdf).

48. B. Wang, P. K. Reville, M. Y. Yassouf, F. Z. Jelloul, C. Ly, P. N. Desai, Z. Wang, P. Borges[†], I. Veletic, E. Dasdemir, J. K. Burks, G. Tang, S. Guo, A. I. Garza, C. Nasnas, N. R. Vaughn, N. Baran, Q. Deng, J. Matthews, P. H. Gunaratne, **D. A. Antunes**, S. Ekmekcioglu, K. Sasaki, M. B. Garcia, B. Cuglievan, D. Hao, N. Daver, M. R. Green, M. Konopleva, A. Futreal, S. M. Post, and H. A. Abbas[∝]. Comprehensive characterization of IFNγ signaling in acute myeloid leukemia reveals prognostic and therapeutic strategies. *Nat Commun*, 15(1):1821, Feb 2024 (pdf).

47. Romanos Fasoulis, Mauricio M Rigo, Gregory Lizée, **D. A. Antunes**, and Lydia E[∝] Kavraki. APE-Gen2.0: Expanding Rapid Class I Peptide-Major Histocompatibility Complex Modeling to Post-Translational Modifications and Noncanonical Peptide Geometries. *Journal of chemical information and modeling*, 64(5):1730–1750, mar 2024 (link).

46. **D. A. Antunes**[∝], B. M. Baker, M. Cornberg, and L. K. Selin. Quantification and prediction of t-cell cross-reactivity through experimental and computational methods. *Front Immunol*, 15, Feb 2024 (link).

45. **D. A. Antunes**[∝], C. T. Schoeder, B. Minkyung, and E. A. Donadi. Editorial: Structural modeling and computational analyses of immune system molecules. *Front Immunol*, 15, Feb 2023 (link).

44. G. Bebis, M. Kato, M. Kohandel, K. Wilkie, **D. A. Antunes**, K. Chen, and J. Dou. Editorial: Advances in mathematical and computational oncology, volume III. *Front Oncol*, 13:1282882, Sep 2023 (link).

43. R. Fasoulis, M. M. Rigo, **D. A. Antunes**, G. Paliouras[∝], and L. E. Kavraki[∝]. Transfer learning improves pMHC kinetic stability and immunogenicity predictions. *Immunoinformatics.*, 13, Dec 2023 (link).

42. A. F. Fonseca[‡] and **D. A. Antunes**[∝]. CrossDome: an interactive R package to predict cross-reactivity risk using immunopeptidomics databases. *Front Immunol*, 14:1142573, Jun 2023 (link).

41. A. Conev, M. M. Rigo, D. Devaurs, A. F. Fonseca[‡], H. Kalavadwala[ψ], M. Vaz de Freitas[‡], C. Clementi, G. Zanatta, **D. A. Antunes**[∝], and L. E. Kavraki[∝]. EnGens: a computational framework for generation and analysis of representative protein conformational ensembles. *Brief Bioinform*, 24(4), Jul 2023 (link).

40. S. Klein, J. Mischke, F. Beruldsen[†], I Prinz, **D. A. Antunes**, M. Cornberg, and A. R. M. Kraft[∝]. T Cell Immune Responses Are Shaped Differently during Chronic Viral Infection. *Pathogens*, 12(5), May 2023 (link).

39. S. Hall-Swan, J. Slone, M. M. Rigo, **D. A. Antunes**, G Lizée, and L. E. Kavraki[∝]. PepSim: T-cell cross-reactivity prediction via comparison of peptide sequence and peptide-HLA structure. *Front Immunol*, 14:1108303, Apr 2023 (link).

38. P. Desai, B. Wang, A F Fonseca[‡], P. Borges[†], F. Jelloul, P. Reville, E. Lee, C. Ly, A. Basi, J. Root, N. Baran, S. Post, Q. Deng, H. Sun, A. Harmanci, J. Burks, J. Gomez, C. DiNardo, N. Daver, G Al-Atrash, M. Konopleva, M. Green, **D. A. Antunes**, F. D. Hao, and H. Abbas[∝]. Single-Cell Profiling of CD8+ T Cells in Acute Myeloid Leukemia Reveals a Continuous Spectrum of Differentiation and Clonal Hyperexpansion. *Cancer Immunol Res*, pages OF1–OF18, Jun 2023 (link).

37. H. M. Sonnemann, B. Pazdrak, **D. A. Antunes**, J. Roszik, and G Lizée[∝]. Vestigial-like 1 (VGLL1): An ancient co-transcriptional activator linking wing, placenta, and tumor development. *Biochim Biophys Acta Rev Cancer*, page 188892, Mar 2023 (link).

36. S. E. Lee, F. Wang, M. Grefe, A. Trujillo-Ocampo, W. Ruiz-Vasquez, K. Takahashi, H. A. Abbas, P. Borges[†], **D. A. Antunes**, G. Al-Atrash, N. Daver, J. J. Molldrem, A. Futreal, G. Garcia-Manero, and J. S. Im[∝]. Immunologic Predictors for Clinical Responses during Immune Checkpoint Blockade in Patients with Myelodysplastic Syndromes. *Clin Cancer Res*, pages OF1–OF14, Mar 2023 (link).

35. C. C. Alves, T. Arns, M. L. Oliveira, P. Moreau, **D. A. Antunes**, E. C. Castelli, C. T. Mendes-Junior, S. Giuliatti, and E. A. Donadi[∝]. Computational and atomistic studies applied to the understanding of the structural and behavioral features of the immune checkpoint HLA-G molecule and gene. *Hum Immunol*, S0198-8859(23)00004-6, Jan 2023 (link).

34. K. R. Jackson[*], **D. A. Antunes**[*], A. H. Talukder, A. R. Maleki, K. Amagai, A. Salmon, A. S. Katailiha, Y. Chiu, R. Fasoulis, M. M. Rigo, J. R. Abella, B. D. Melendez, F. Li, Y. Sun, H. M. Sonnemann, V. Belousov, F. Frenkel, S. Justesen, A. Makaju, Y. Liu, D. Horn, D. Lopez-Ferrer, A. F. Huhmer, P. Hwu, J. Roszik, D. Hawke, L. E. Kavraki, and G. Lizée[∝]. Charge-based interactions through peptide position 4 drive diversity of antigen presentation by human leukocyte antigen class I molecules. *PNAS Nexus*, 1(3):pgac124, Jul 2022 (pdf).

33. M. M. Rigo, R. Fasoulis, A. Conev, S. Hall-Swan, **D. A. Antunes**[∝], and L. E. Kavraki[∝]. SARS-Arena: Sequence and Structure-Guided Selection of Conserved Peptides from SARS-related Coronaviruses for Novel Vaccine Development. *Front Immunol*, 13:931155, Jul 2022 (link).

32. A. Conev, D. Devaurs, M. M. Rigo, **D. A. Antunes**[∝], and L. E. Kavraki[∝]. 3pHLA-score improves structure-based peptide-HLA binding affinity prediction. *Sci Rep*, 12(1):10749, Jun 2022 (pdf).

31. N. Sapoval, A. Aghazadeh, M. G. Nute, **D. A. Antunes**, A. Balaji, R. Baraniuk, C. J. Barberan, R. Dannenfelser, C. Dun, M. Edrisi, R. A. L. Elworth, B. Kille, A. Kyrillidis, L. Nakhleh, C. R. Wolfe, Z. Yan, V. Yao, and T. J.

Treangen$^{\propto}$. Current progress and open challenges for applying deep learning across the biosciences. *Nat Commun*, 13(1):1728, Apr 2022 (pdf).

30. D. Devaurs$^{\propto}$, **D. A. Antunes**, and A. J. Borysik$^{\propto}$. Computational Modeling of Molecular Structures Guided by Hydrogen-Exchange Data. *J Am Soc Mass Spectrom*, 33(2):215–237, Feb 2022 (pdf).

29. R. F. Tarabini, M. M. Rigo, A. F. Fonseca‡, F. Rubin, R. Bellé, L. E. Kavraki, T. C. Ferreto, **D. A. Antunes**$^{\propto}$, and A. P. D. de Souza$^{\propto}$. Large-Scale Structure-Based Screening of Potential T Cell Cross-Reactivities Involving Peptide-Targets From BCG Vaccine and SARS-CoV-2. *Front Immunol*, 12:812176, Jan 2021 (link).

28. S. Hall-Swan, D. Devaurs, M. M. Rigo, **D. A. Antunes**$^{\propto}$, L. E. Kavraki$^{\propto}$, and G. Zanatta$^{\propto}$. DINC-COVID: A webserver for ensemble docking with flexible SARS-CoV-2 proteins. *Comput Biol Med*, 139:104943, Dec 2021 (pdf).

27. J. R. Abella, **D. A. Antunes**, K. Jackson, G. Lizée, C. Clementi, and L. E. Kavraki$^{\propto}$. Markov state modeling reveals alternative unbinding pathways for peptide–mhc complexes. *Proceedings of the National Academy of Sciences (PNAS)*, 117(48):30610–30618, Dec 2020 (pdf).

26. T. Arns, **D. A. Antunes**, J. R. Abella, M. M. Rigo, L. E. Kavraki, S. Giuliatti, and E. A. Donadi$^{\propto}$. Structural modeling and molecular dynamics of the immune checkpoint molecule HLA-G. *Frontiers in Immunology*, 11:2882, Nov 2020 (pdf).

25. **D. A. Antunes**, J. R. Abella, S. Hall-Swan, D. Devaurs, A. Conev, M. Moll, G. Lizée, and L. E. Kavraki$^{\propto}$. HLA-Arena: a customizable environment for the structural modeling and analysis of peptide-HLA complexes for cancer immunotherapy. *JCO Clinical Cancer Informatics*, 4:623–636, July 2020 (pdf).

24. D. Devaurs, **D. A. Antunes**, and L. E. Kavraki$^{\propto}$. Computational analysis of complement inhibitor compstatin using molecular dynamics. *J. Mol. Model.*, 26(9):231, Aug 2020 (pdf).

23. J. R. Abella, **D. A. Antunes**, C. Clementi, and L. E. Kavraki$^{\propto}$. Large-scale structure-based prediction of stable peptide binding to Class I HLAs using random forests. *Front. Immunol.*, 11(1583), July 2020 (pdf).

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$^{\propto}$. Hepatitis E Virus (HEV)-Specific T Cell Receptor Cross-Recognition: Implications for Immunotherapy. *Front. Immunol.*, 10:2076, Sep 2019 (pdf).

21. D. Devaurs, **D. A. Antunes**, S. Hall-Swan, N. Mitchell, M. Moll, G. Lizée, and L. E. Kavraki$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. 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. D. Devaurs, **D. A. Antunes**, and Lydia E. Kavraki$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. Coarse-Grained Conformational Sampling of Protein Structure Improves the Fit to Experimental Hydrogen-Exchange Data. *Front. Mol. Biosci.*, 4:13, 2017
13. D. Devaurs, M. Papanastasiou, **D. A. Antunes**, J. R. Abella, M. Moll, D. Ricklin, J. D. Lambris, and L. E. Kavraki$^{\propto}$. 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$^{\propto}$. Improved structural method for T-cell cross-reactivity prediction. *Mol. Immunol.*, 67(2 Pt B):303–310, Oct 2015
11. **D. A. Antunes**, D. Devaurs, and L. E. Kavraki$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. Lessons from molecular modeling human α-L-iduronidase. *J. Mol. Graph. Model.*, 54:107–113, Nov 2014
7. **D. A. Antunes**, M. M. Rigo, M. Sinigaglia, R. M. de Medeiros, D. M. Junqueira, S. E. Almeida, and G. F. Vieira$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. Immunogenic epitopes of Hantaviruses' N protein are restricted to conserved regions. *Front. Biosci. (Landmark)*, 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$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. 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$^{\propto}$. 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 *Anals 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 *Anals 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 *Anals 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$^{\propto}$. 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

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).

Selected Poster Abstracts (out of a total of 59 posters presented in conferences before joining UH)

- D.A. Antunes, J.R. Abella, S. Hall-Swan, D. Devaurs, A. Conev, M. Moll, G. Lizée, and L.E. Kavraki. HLA-Arena: Enabling structure-based virtual screening of tumor-associated antigens for immunotherapy. Virtual, March 2021. 2021 Future of Immunology Research Symposium

- **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**)

Poster Abstracts and Oral Presentations by Trainees (from after joining UH as an Asssistant Professor)

64. J.D. Lewis, M.V. Freitas, and D.A. Antunes. Improving cancer vaccine design for Black and Latine patients. Gulf Coast Consortium, Houston, TX, December 2025. Gulf Coast Consortium Cellular and Molecular Biophysics Trainee Seminar Series. **Oral Presentation**
63. E. Dasdemir, I. Veletic, C. P. Ly, A. E. Quesada, C. D. Pacheco, F. Z. Jelloul, P. Borges, S. Basu, S. Jindal, Z. Wang, A. Lazar, K. M. Wani, D. A. Antunes, P. K. Reville, P. H. Gunaratne, R. J. Tower, P. Sharma, and H. A. Abbas. Integrative spatial multi-omics reveals niche-specific inflammatory signaling and differentiation hierarchies in acute myeloid leukemia. Orange County Convention Center in Orlando, Florida, December 2025. American Society of Hematology (ASH) 2025 Annual Meeting. **Poster Presentation**
62. F. Alexander A. Beruldsen and D.A. Antunes. Mathematical modeling of interclonal t-cell competition reveals impact of suboptimal clones on tumor clearance. December 2025. Poster Presentation
61. S.E Choi, M. Freitas, R.L. Belle, D. Devaurs, T.C. Ferreto, and D. Antunes. Large-scale modeling of phla complexes for structure-based immunogenicity prediction. Gaylord National Resort and Convention Center in National Harbor, MD, November 2025. The Society for Immunotherapy of Cancer's 40th Anniversary Annual Meeting (SITC). Poster Presentation
60. J.D. Lewis, M.V. Freitas, and D.A. Antunes. Improving cancer vaccine design for African American and Latine patients with PIK3CA-associated breast cancer. Center for Nuclear Receptors and Cell Signaling, University of Houston, Houston, TX, November 2025. Center for Nuclear Receptors and Cell Signaling Seminar Series. **Oral Presentation**
59. J.D. Lewis, M.V. Freitas, and D.A. Antunes. Improving cancer vaccine design for African American and Latine Patients. Gaylord National Resort and Convention Center in National Harbor, MD, November 2025. The Society for Immunotherapy of Cancer's 40th Anniversary Annual Meeting (SITC). **Poster Presentation**
58. P. Borges, M.V. Freitas, S. Ullah, H. A. Abbas, and D.A. Antunes. Structure-guided design and repertoire clustering of t cell receptors targeting an aml neoantigen. Gaylord National Resort and Convention Center in National Harbor, MD, November 2025. The Society for Immunotherapy of Cancer's 40th Anniversary Annual Meeting (SITC). Poster Presentation
57. M.V. Freitas and D.A. Antunes. HLA-Arena 2.0: Expanding access to phla structural modeling and peptide prioritization for precision immunotherapy. Gaylord National Resort and Convention Center in National Harbor, MD, November 2025. The Society for Immunotherapy of Cancer's 40th Anniversary Annual Meeting (SITC). Poster Presentation
56. M.V. Freitas and D.A. Antunes. Structure-guided cancer immunotherapy design with HLA-Arena and Cross-Dome. National Cancer Institute, Rockville, MD, August 2025. NIH/NCI Informatics Technology for Cancer

Research (ITCR) Annual Meeting. **Oral Presentation**

55. F. Beruldsen, M.V. Freitas, and D.A. Antunes. Flipbook & RMSX: Publication ready molecular visualizations. National Cancer Institute, Rockville, MD, August 2025. NIH/NCI Informatics Technology for Cancer Research (ITCR) Annual Meeting. Poster Presentation

54. F. Beruldsen, M.V. Freitas, and D.A. Antunes. Flipbook & RMSX: Tools to see when and where proteins move during md simulations. National Cancer Institute, Rockville, MD, August 2025. NIH/NCI Informatics Technology for Cancer Research (ITCR) Annual Meeting. **Oral Presentation**

53. M.V. Freitas, A. Borigi, V. J. Huang, J. D. Lewis, and D.A. Antunes. Ai-driven scoring for virtual screening of peptide-based ligands. Student Center South, University of Houston, Houston, TX, April 2025. Drug Discovery Institute (DDI) Symposium. Poster Presentation

52. A. Trujillo-Ocampo, M. Grefe, P. Borges, J. Clinton, H. He, D. Li, L. Yu, M. Vaz de Freitas, L. St. John, K. Clise-Dwyer, G. Alatrash, D.A. Antunes, Q. Ma, J.J. Molldrem, E.J. Shpall, and Im J.S. Cord-derived invariant natural killer t cells as novel cell therapy to improve the outcome of hematopoietic stem cell transplantation. San Diego, CA, December 2024. The 66th ASH Annual Meeting Abstracts. Poster Presentation

51. P. Borges, M.V. Freitas, and D.A. Antunes. Advancing pipelines for T-cell off-target toxicity prediction using CrossDome. Bioscience Research Collaborative Rice University, Houston, TX, November 2024. 34th Keck Annual Research Conference: Machine Learning and Computation in Structural Biology. Poster Presentation

50. P. Borges, M.V. Freitas, A. Trujilo-Ocampo, M. Grefe, J. Shpall, E. Im, and D.A. Antunes. Single-cell rna and tcr sequence analysis of adult and cord-derived invariant natural killer T-cells reveal two distinct functional subset. Bioscience Research Collaborative Rice University, Houston, TX, October 2024. GCC Single Cell & Spatial Omics Symposium. Poster Presentation

49. J. Lewis, M. V. Freitas, and D. A. Antunes. Improving the design of cancer vaccines targeting PIK3CA-associated antigens for underrepresented minority patients. Phoenix Convention Center, Phoenix, AZ, October 2024. National Diversity in STEM Conference SACNAS 2024. Poster Presentation

48. V. M. Maranholkar, S. Nandy, M.V. Freitas, B. Vu, K. Kourentzi, D.A. Antunes, M. Sen, and R. Willson. What is protein A? Natural variation in IgG-binding proteins. San Diego Convention Center, Hilton San Diego Bayfront, San Diego, CA, October 2024. Poster Presentation

47. V.J Huang, M.V. Freitas, and D.A. Antunes. Molecular docking analysis of peptide-protein interactions for consensus scoring and binding affinity prediction. Baltimore, Maryland, October 2024. 2024 BMES Annual Meeting, BMES High School Poster Expo. High School Poster Presentation

46. M.V. Freitas and D.A. Antunes. HLA-Arena 2.0: Upgrading structural modeling and analysis for cancer immunotherapy. The Eiteljorg Museum, Indianapolis, In, September 2024. NIH/NCI Informatics Technology for Cancer Research (ITCR) Annual Meeting. **Oral Presentation**

45. P. Borges, M.V. Freitas, and D.A. Antunes. Developing new pipelines for T-cell off-target toxicity prediction with CrossDome. The Eiteljorg Museum, Indianapolis, In,, September 2024. NIH/NCI Informatics Technology for Cancer Research (ITCR) Annual Meeting. Poster Presentation

44. S.E. Choi, T. Arns, M. Vaz de Freitas, H.N. Le, S. Giuliatti, E. A. Donadi, and D.A. Antunes. HLA-G7: revealing possible “HLA-like” dimer through molecular modeling. University of Texas Medical Branch, Galveston, TX, April 2024. Sealy Center’s Structural Biology Annual Symposium. Poster Presentation

43. J.D. Lewis, R. Fasoulis, S. Tran, A. Conev, S. Hall-Swan, L.E. Kavraki, and D.A. Antunes. Investigating the accuracy of diverse scoring functions on ranking peptide-HLA conformations. University of Texas Medical Branch, Galveston, TX, April 2024. Sealy Center’s Structural Biology Annual Symposium. Poster Presentation

42. F. Beruldsen, M. Vaz de Freitas, and D.A. Antunes. Combining the best features of RMSD and RMSF: RMSX, showing when and where changes happen in molecular dynamic simulations investigating the accuracy of diverse scoring functions on ranking peptide-HLA conformations. University of Texas Medical Branch, Galveston, TX, April 2024. Sealy Center's Structural Biology Annual Symposium. Poster Presentation

41. P. Borges, H. Abbas, and D.A. Antunes. Insights into immune-malignant cell interplay in acute myeloid leukemia: Deciphering TCR repertoire dynamics and therapeutic implications. 6500 Main St, Houston, TX, April 2024. Gulf Coast Consortia 4th Annual Future of Immunology Symposium. Poster Presentation, Lightning Talk Presentation

40. H.N. Le, M. Vaz de Freitas, and D.A. Antunes. Dynamic contact analysis of TCRpHLA complexes. 6500 Main St, Houston, TX, April 2024. Gulf Coast Consortia 4th Annual Future of Immunology Symposium. Poster Presentation

39. A. Borigi, M. Vaz de Freitas, J.D. Lewis, and D.A. Antunes. Enhancing protein data analysis: Automated bot deployment for efficient peptide screening. MD Anderson Library, University of Houston, Houston, TX, March 2024. BSGS Annual Symposium. Poster Presentation

38. M. Vaz de Freitas and D.A. Antunes. HLA-Arena 2.0: Next-generation structural modeling and analysis for cancer immunotherapy. CNRCS, University of Houston, Houston, TX, February 2024. CNRCS Annual Symposium. **Oral Presentation**

37. H.N. Le, M. Vaz de Freitas, and D.A. Antunes. Simulation-based determination of molecular fingerprints driving t-cell specificity. CNRCS, University of Houston, Houston, TX, February 2024. CNRCS Annual Symposium. **Oral Presentation**

36. A. Calderon-Macedo, M. Vaz de Freitas, M. L. Goldberg, and D.A. Antunes. Notes on conducting metal molecular simulations using Gromacs-2021 and CHARMM36 force field. CNRCS, University of Houston, Houston, TX, February 2024. CNRCS Annual Symposium. Poster Presentation

35. J.D. Lewis, S. Shabahang, G. Cuny, and D.A. Antunes. Examining the dynamic interactiknd of drug activators for the pseudokinase MLKL. CNRCS, University of Houston, Houston, TX, February 2024. CNRCS Annual Symposium. Poster Presentation

34. M. Vaz de Freitas, H.N. Le, and D.A. Antunes. Simulation-based determination of molecular fingerprints driving t-cell specificity. 6500 Main St, Houston, TX, November 2023. Gulf Coast Consortia Cellular and Molecular Biophysics Conference. Poster Presentation, Lightning Talk Presentation

33. M. Vaz de Freitas and D.A. Antunes. Ensemble generator and docking approaches for accelerated drug discovery. CNRCS, University of Houston, Houston, TX, November 2023. CNRCS seminars 2023. **Oral Presentation**

32. S. Tran, J. Lewis, A. Borigi, M. Vaz de Freitas, and D.A. Antunes. Benchmarking alternative scoring functions' ranking ability for peptide ligands. 6500 Main St, Houston, TX, November 2023. Gulf Coast Consortia Cellular and Molecular Biophysics Conference. Poster Presentation

31. J.D. Lewis, A. Conev, M. Vaz de Freitas, S. Hall-Swan, L.E. Kavraki, and D.A. Antunes. Determining the accuracy of alternative scoring functions for docking peptides to HLA receptors. Oregon Convention Center, Portland, Oregon, October 2023. SACNAS NDiSTEM Annual Conference. Poster Presentation

30. H.N. Le, M.V. Freitas, A.F. Fonseca, and D.A. Antunes. Identification of molecular features driving molecular mimicry in T-cell-based antigen recognition. Dell Medical School - Health Learning Building, UT, Austin, TX, April 2023. Expanding Texas Leadership in Computational Oncology Throughout the Cancer Continuum: A CPRIT Symposium. Poster Presentation

29. P. Borges, S. Lee, F. Wang, M. Grefe, A. Trujillo-Ocampo, W. Ruiz-Vasquez, K. Takahashi, H. Abbas, G. Al-Atrash, N. Daver, J.J. Molldrem, A. Futreal, G. Garcia-Manero, J.S. Im, and D.A. Antunes. Analysis of the

TCR repertoire of myelodysplastic syndrome patients treated with immunotherapies. Dell Medical School - Health Learning Building, UT, Austin, TX, April 2023. Expanding Texas Leadership in Computational Oncology Throughout the Cancer Continuum: A CPRIT Symposium. **Oral Presentation**

28. J.D. Lewis, S. Shabahang, G. Cuny, and D.A. Antunes. Analyzing dynamic interactions of drug activators for the pseudokinase MLKL. Levin Hall at the University of Texas Medical Branch, Galveston, TX, April 2023. Annual Sealy Center for Structural Biology Symposium. Poster Presentation

27. P.N. Desai, B. Wang, A.F. Fonseca, P. Borges, F.Z. Jelloul, P.K. Reville, C. Ly, J. Root, A. Basi, E. Lee, N. Baran, S. Post, Q. Deng, H. Sun, A. Harmanci, J. Burks, J. Gomez, C. DiNardo, N. Daver, G. Al-Atrash, M. Konopleva, M.R. Green, D.A. Antunes, A. Futreal, D. Hao, and H.A. Abbas. Paired single cell transcriptomic and repertoire profiling of CD8 cells in acute myeloid leukemia reveals distinct functional states at time of diagnosis and therapy resistance that informs patient outcomes. Orange County Convention Center, Orlando, Florida, April 2023. AACR Annual Meeting

26. P. Borges, S. Lee, F. Wang, M. Grefe, A. Trujillo-Ocampo, W. Ruiz-Vasquez, K. Takahashi, H. Abbas, G. Al-Atrash, N. Daver, A. Molldrem, J.J.and Futreal, G. Garcia-Manero, J.S. Im, and D.A. Antunes. Low prevalence of known "public"TCRs in myelodysplastic syndrome patients treated with immunotherapies. Elizabeth D. Rockwell Pavilion University of Houston, Houston, TX, March 2023. Bioscience Graduate Society 14th Annual Graduate Student Symposium. **Oral Presentation**

25. J.D. Lewis, A. Conev, M.V. Freitas, S. Hall-Swan, L.E. Kavraki, , and D.A Antunes. Examining the accuracy of alternative scoring functions on the ranking of docked peptide-HLA conformations. Elizabeth D. Rockwell Pavilion University of Houston, Houston, TX, March 2023. Bioscience Graduate Society 14th Annual Graduate Student Symposium. Poster presentation

24. S.E. Choi, K.R. Jackson, A.H. Talukder, A.R. Maleki, K. Amagai, A. Salmon, A.S. Katailiha, Y. Chiu, R. Fasoulis, M.M. Rigo, J.R. Abella, B.D. Melendez, F. Li, Y. Sun, H.M. Sonnemann, V. Belousov, F. Frenkel, S. Justesen, A. Makaju, Y. Liu, D. Horn, D. Lopez-Ferrer, A.F. Hummer, P. Hwu, J. Roszik, D. Hawke, L.E. Kavraki, G. Lizée, and D.A. Antunes. Investigating the role of position 4 on the binding of peptides to HLA-A02:01 and HLA-A24:02. Elizabeth D. Rockwell Pavilion University of Houston, Houston, TX, March 2023. Bioscience Graduate Society 14th Annual Graduate Student Symposium. Poster presentation

23. J.D. Lewis, A. Conev, M. Vaz de Freitas, S. Hall-Swan, L.E. Kavraki, and D.A. Antunes. Examining the accuracy of alternative scoring functions on the ranking of docked peptide-HLA conformations. MD Anderson Library, University of Houston, Houston, TX, March 2023. Bioscience Graduate Society. Poster Presentation

22. J.D. Lewis, S. Hall-Swan, A. Conev, A.F. Fonseca, M.V. Freitas, L.E. Kavraki, and D.A. Antunes. Investigating the accuracy of alternative scoring functions on the ranking of docked peptide-HLA conformations. Bioscience Research Collaborative Rice University, Houston, TX, March 2023. 3rd Annual GCC Future of Immunology Symposium. Poster presentation

21. H.N. Le, M.V. Freitas, and D.A. Antunes. Structural modeling of t-cell receptor interactions for immunotherapy applications. Bioscience Research Collaborative Rice University, Houston, TX, March 2023. 3rd Annual GCC Future of Immunology Symposium

20. J.D. Lewis, A. Conev, M. Vaz de Freitas, A.F. Fonseca, S. Hall-Swan, L.E. Kavraki, and D.A. Antunes. Assessing the accuracy of alternative scoring functions on the ranking of peptide-HLA conformations. Center for Nuclear Receptors and Cell Signaling, University of Houston, Houston, TX, December 2022. Center for Nuclear Receptors and Cell Signaling Annual Symposium. Poster Presentation

19. P. Borges, P. Malaney, S. Post, D.A. Antunes, and H. Abbas. The role of Chr7/7q deletion in AML cells. CNRCS University of Houston, Houston, TX, December 2022. CNRCS Annual Symposium. Poster presentation

18. H.N. Le, C. Soon, F. Beruldsen, A.F. Fonseca, M. Cornberg, and D.A. Antunes. Analysis of t-cell receptor

interactions reveals alternative recognition of HEV-derived peptides. CNRCS University of Houston, Houston, TX, December 2022. CNRCS Annual Symposium. Poster presentation

17. A.F. Fonseca and D.A. Antunes. CrossDome: An interactive r package to predict T-cell cross-reactivity risk on immunopeptidomics databases. Boston, MA, November 2022. Society for Immunotherapy of Cancer - SITC
16. S.E. Choi, T. Arns, H.N. Le, M.V. Freitas, S. Giuliatti, E.A. Donadi, and D.A. Antunes. Molecular modeling reveals alternative dimer possibilities for HLA-G7 molecules. BioScience Research Collaborative Center, Rice University, Houston, TX, October 2022. Keck Annual Research Conference. Poster Presentation
15. J. Lewis, S. Hall-Swan, A. Conev, A.F. Fonseca, M.V. Freitas, L.E. Kavraki, and D.A. Antunes. Evaluating the ranking power of peptide-HLA scoring functions. BioScience Research Collaborative Center, Rice University, Houston, TX, October 2022. 32nd Annual Keck Conference; Structural Biology: Past, Present, Future. Poster Presentation
14. S.E. Choi, T. Arns, H.N. Le, M.V. Freitas, S. Giuliatti, E.A. Donadi, and D.A. Antunes. Molecular modeling reveals alternative dimer possibilities for HLA-G7 molecules. Bioscience Research Collaborative Rice University, Houston, TX, October 2022. 32nd Keck Annual Research Conference Structural Biology: Past, Present, and Future. Poster presentation
13. P. Borges, P. Malaney, Y. Sun, S. Post, D.A. Antunes, and H. Abbas. The role of Chr7/7q deletion in AML cells. Bioscience Research Collaborative Rice University, Houston, TX, October 2022. 32nd Keck Annual Research Conference Structural Biology: Past, Present, and Future. Poster presentation
12. H.N. Le, C. Soon, F. Beruldsen, A.F. Fonseca, M. Cornberg, and D.A. Antunes. Alternative recognition patterns driving cross-genotype response with hepatitis e virus-specific T cells. Bioscience Research Collaborative Rice University, Houston, TX, October 2022. 32nd Keck Annual Research Conference Structural Biology: Past, Present, and Future. Poster presentation
11. J. Lewis, S. Hall-Swan, A. Conev, A.F. Fonseca, M.V. Freitas, L.E. Kavraki, and D.A. Antunes. Evaluation of the ranking power of peptide-HLA scoring functions. Bioscience Research Collaborative Rice University, Houston, TX, October 2022. 32nd Keck Annual Research Conference Structural Biology: Past, Present, and Future. Poster presentation
10. F. Beruldsen, A.F. Fonseca, and D.A. Antunes. Enabling large-scale modeling of immune complexes with webserver automation using selenium. Bioscience Research Collaborative Rice University, Houston, TX, October 2022. 32nd Keck Annual Research Conference Structural Biology: Past, Present, and Future. Poster presentation
9. A.F. Fonseca and D.A. Antunes. Leveraging structural data on contact maps to improve T-cell cross-reactivity predictions. Bioscience Research Collaborative Rice University, Houston, TX, October 2022. 32nd Keck Annual Research Conference Structural Biology: Past, Present, and Future. Poster presentation
8. R. Fasoulis, M.M. Rigo, D.A. Antunes, and L.E. Kavraki. Ape-Gen2.0: A web server for generating ensembles of peptide conformations bound to MHC receptors. EPNEC Washington University School of Medicine in St. Louis, St. Louis, MO, September 2022. NCI Informatics Technology for Cancer Research
7. M.M. Rigo, A. Conev, R. Fasoulis, D.A. Antunes, G. Lizée, and L.E. Kavraki. PROTEAN-CR: A proteomics toolkit for ensemble analysis in cancer research. EPNEC Washington University School of Medicine in St. Louis, St. Louis, MO, September 2022. NCI Informatics Technology for Cancer Research
6. A. Conev, D. Devaurs, M.M. Rigo, D.A. Antunes, and L.E. Kavraki. 3pHLA-score: improved structure-based peptide-HLA binding affinity prediction. EPNEC Washington University School of Medicine in St. Louis, St. Louis, MO, September 2022. NCI Informatics Technology for Cancer Research
5. D. Devaurs, D.A. Antunes, and A.J. Borysik. Computational modeling of molecular structures guided by experimental HDX-MS data. London, UK, April 2022. International Conference on Hydrogen-Deuterium Exchange

Mass Spectrometry (HDX-MS)

4. A.F. Fonseca and D.A. Antunes. CrossDome: An R package to measure T-cell cross-reactivity risk. Virtual, December 2021. Center for Nuclear Receptors and Cell Signaling Virtual Symposium
3. F. Beruldsen, C. Soon, A.F. Fonseca, M. Cornberg, and D.A. Antunes. Explaining directionality in T-cell cross-reactivity between HEV genotypes. Virtual, December 2021. Center for Nuclear Receptors and Cell Signaling Virtual Symposium. Poster presentation
2. J. Lewis, S. Hall-Swan, A. Conev, A.F. Fonseca, L.E. Kavraki, and D.A. Antunes. Evaluation of scoring functions to rank bound conformations of peptide-HLA complexes. Virtual, December 2021. Center for Nuclear Receptors and Cell Signaling Virtual Symposium. Poster presentation
1. S.E. Choi, A.F. Fonseca, K.R. Jackson, G. Lizée, and D.A. Antunes. Uncovering the role of proline as a source of increased stability for peptide-HLA complexes. Virtual, December 2021. Center for Nuclear Receptors and Cell Signaling Virtual Symposium. Poster presentation

AWARDS AND HONORS BY ANTUNES LAB TRAINEES

2023	Best Poster award at 50th Annual NDiSTEM Conference for (SACNAS) (Portland, Oregon)	Jayla Lewis
2023	Acceptance to the HEALTH-RCMI Professional Development Program (UH, Houston)	Martiela Freitas
2023	Best Poster award at 27th Structural Biology Annual Symposium (UTMB, Galveston)	Jayla Lewis
2023	Best Poster award at 14th Annual Graduate Student Symposium (UH, Houston)	Sae Hee Choi
2022	Best Poster award at CNRCS Annual Research Symposium (UH, Houston)	Jayla Lewis
2021	Best Poster award at CNRCS Annual Research Symposium (UH, Houston)	André Fonseca

CONTRIBUTED SOFTWARE

RMSX and Flipbook: a simple-to-understand and simple-to-implement tool for visualizing and quantifying time-resolved residue-specific motions in molecular dynamics simulations, by integrating RMSD and RMSF data. (https://github.com/AntunesLab/rmsx). Role: PI.

CrossDome: an interactive R package to predict cross-reactivity risk using immunopeptidomics databases. (https://github.com/AntunesLab/crossdome). Role: PI.

EnGens: a computational framework for generation and analysis of representative protein conformational ensembles. (https://github.com/KavrakiLab/EnGens). Role: Co-PI.

DINC-COVID: a webserver for ensemble docking with SARS-CoV-2 proteins. (http://dinc-covid.kavrakilab.org/). Role: Co-PI.

3pHLA-score: improved structure-based peptide-HLA binding affinity prediction. (https://github.com/KavrakiLab/3pHLA-score). Role: Co-PI.

SARS-Arena: selection of conserved peptides from SARS-related Coronaviruses for Novel Vaccine Development. (https://github.com/KavrakiLab/SARS-Arena). Role: Co-PI.

HLA-Arena: a customizable environment for structure-based analysis in cancer immunotherapy. (https://github.com/KavrakiLab/hla-arena). Role: first author/key personnel.

DINC: a webserver for incremental meta-docking of large ligands. (http://dinc.kavrakilab.org/) Role: first author/key personnel.

TL-MHC: transfer learning for pMHC kinetic stability and immunogenicity predictions. (https://github.com/KavrakiLab/TL-MHC). Role: key personnel.

pHLA-RF: random forest classifier to predict HLA binders using APE-Gen models. (https://github.com/KavrakiLab/pHLA-RFclassifier-from-structure). Role: key personnel.

PepSim: comparison of peptide sequence and peptide-HLA structure for T-cell cross-reactivity predictions. (https://pepsim.kavrakilab.org). Role: key personnel.

APE-Gen2.0: fast and accurate pMHC modeling accounting for PTMs and noncanonical geometries. (https://apegen.kavrakilab.org/). Role: key personnel.

APE-Gen: a fast method for generating ensembles of bound pMHC conformations. (http://github.com/KavrakiLab/APE-Gen). Role: key personnel.

DockTope: a webserver for docking-based structural prediction of pMHC complexes. (http://tools.iedb.org/docktope/). Role: key personnel.

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

FUNDED RESEARCH PROJECTS: PI, CO-PI OR COLLABORATOR

Development and optimization of mRNA vaccines using artificial intelligence methods. Project supported by the National Council for Scientific and Technological Development (CNPq – Brazil). **Role**: Co-I. **Total Funding**: US$ 89,244.48. Start date: 01-01-2025. End date: 12-31-2026.

Structure-guided cancer immunotherapy design with HLA-Arena and CrossDome. NIH/R21 grant funded by NCI Informatics Technology for Cancer Research (ITCR) Program (1R21CA289333-01). **Role**: PI. **Total Funding**: US$ 414,649. **Total Direct Cost**: US$ 285,907. Start date: 07-01-2024. End date: 06-30-2026.

Improving the design of immunotherapies for underrepresented minorities. Project supported by a HEALTH-RCMI Pilot Grant Program, with funding from the National Institute on Minority Health and Health Disparities (NIMHD/NIH), under award number U54MD015946. **Role**: PI. **Total Funding**: US$ 77,500.00. **Total Direct Cost**: US$ 50,000.00. Start date: 03-01-2024. End date: 02-28-2025.

Integrating new structure-based analysis into tumor-associated antigen discovery pipelines. Set Aside funds corresponding to 10% of the annual budget of the NIH/U01 grant (1U01CA258512-01) funded by NCI Informatics Technology for Cancer Research (ITCR) Program. **Role**: Collaborator. **Total Funding**: US$ 48,000. **Antunes Lab funding**: US$ 48,000. Start date: 10-3-2023. End date: 9-11-2024.

AI-driven scoring for virtual screening of peptide-based ligands. Project supported by the University of Houston Drug Discovery Institute (DDI). **Role**: PI. **Total Funding**: US$ 68,264. **Antunes Lab funding**: US$ 68,264. Start date: 6-1-2023. End date: 12-31-2024.

Structural modeling and analysis of peptide-HLA complexes for cancer immunotherapy applications. High-performance computing start-up grant allocation awarded by the Extreme Science and Engineering Discovery Environment (XSEDE). Project number BIO220107. **Role**: PI. Allocations: (i) 2,500.0 GPU-hours at the San Diego Super Computer (SDSC) Dell Cluster, (ii) 1,600 Node-hours at the Texas Advanced Computing Center (TACC) Stampede2 cluster, and (iii) 50,000 Core-hours at the SDSC AMD Rome cluster. Start date: 8-4-2022. End date: 8-3-2023.

Mixed lineage kinase domain-like (MLKL) protein activators for cancer therapy. Project supported by University of Houston High Priority Area Research Seed Grants 2021-2022. **Role**: Co-PI. **Total Funding**: US$ 70,000. **Antunes Lab funding**: US$ 36,000. Start date: 5-14-2022. End date: 11-1-2023.

FUNDED RESEARCH PROJECTS: KEY PERSONNEL

PROTEAN-CR: Proteomics Toolkit for Ensemble Analysis in Cancer Research. Project supported by NIH, grant number 1U01CA258512-01, through the Informatics Technology for Cancer Research (ITCR) initiative of the National Cancer Institute (NCI). **Role**: Co-author of the proposal and collaborator for the execution of the project. **Total Funding**: US$ 402,077.

Structure-based identification of SARS-derived peptides with potential to induce broad protective immunity. Project supported by NSF, award number 2033262, through Program Solicitation NSF 18-595 (IIBR:RAPID). Role: Co-author of the proposal and collaborator on the execution of the project. **Total Funding**: US$ 119,747.

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 (≈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.

OTHER EXPERIENCE AND PROFESSIONAL MEMBERSHIPS

- Member of the Society for the ImmunoTherapy of Cancer (SITC), 2025 – to date
- Editorial Board Member for Discover Immunity (Springer), 2024 - to date.
- Associate Editor for Front. Molecular Biosciences, section Biological Modeling and Simulation, 2023 – to date
- Reviewer Editor for Front. Molecular Biosciences, section Biological Modeling and Simulation, 2022 – 2023
- Guest Editor in Cancer Genetics, Front. Immunology, collection in computational oncology, 2021 – 2023
- Guest Editor in Systems Immunology, Front. Immunology, collection in modeling immune molecules, 2021 – 2023
- Guest Editor in T Cell Biology, Front. Immunology, collection in T-cell cross-reactivity, 2021 – to date
- Associate Editor for Front. Bioinformatics, Protein Bioinformatics Section, 2021 – to date
- Guest Editor for Antibiotics, collection in Structures and functions of antimicrobial peptides, 2021
- Member of the American Association for the Advancement of Science (AAAS), 2020 – to date
- 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 – 2020
- 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

ACADEMIC SERVICES

Service at Division and Department

- Faculty search committee B&B Dept. (Translational Immunology search), University of Houston, 2024.
- Biochemistry Division Advising session, Fall 2024 Graduate Student Orientation, 2024.
- Biochemistry Division Advising session, Spring 2024 Graduate Student Orientation, 2024.
- Biochemistry Division Advising session, Fall 2023 Graduate Student Orientation, 2023.
- Ad Hoc BCHS Grad. Curriculum Committee, Biochemistry Division, B&B Dept., University of Houston, 2023.
- Faculty search committee B&B Dept. (Protein or Nucleic Acids Biochemistry search), University of Houston, 2023.

- Graduate student recruitment committee (GRAC), 2022 – to present.
- Faculty search committee B&B Dept. (Cancer Biology search), University of Houston, 2021.

Service at College and University

- Served on a Faculty Panel on "Charting Your Course: Navigating Faculty Life at UH", during the 2024 New Faculty Orientation. Conrad Ballroom at the UH Hilton Hotel. August 13, 2024.
- Served on a virtual NSM academic honesty panel, as an NSM Faculty member. June 27, 2023.

Committe Member for Conferences

- Program Committee Member for the *2025 IEEE International Conference on Bioinformatics and Biomedicine* (BIBM'25). Wuhan, China. December 15-18 2025.
- Chair of the Committee for the *CNRCS Annual Research Symposium.* Department of Biology and Biochemistry, College of Natural Sciences and Mathematics, University of Houston. Houston, TX. February 2024.
- Program Committee Member for the *2024 IEEE International Conference on Bioinformatics and Biomedicine* (BIBM'24). Lisbon, Portugal. December 3-6 2024.
- Program Committee Member for the *2023 IEEE International Conference on Bioinformatics and Biomedicine* (BIBM'23). Istanbul, Turkey. December 5-8 2023.
- Program Committee Member for the *CNRCS Annual Research Symposium.* Department of Biology and Biochemistry, College of Natural Sciences and Mathematics, University of Houston. Houston, TX. December 2022.
- Program Committee Member for the *CNRCS Annual Research Symposium.* Department of Biology and Biochemistry, College of Natural Sciences and Mathematics, University of Houston. Houston, TX. December 2021.
- Chair of the session on *General cancer computational biology* at the *Third International Symposium on Mathematical and Computational Oncology* (ISMCO'21). Virtual. October 2021.
- Chair of the session on *General cancer computational biology*, and the *Poster session I*, at the *Second International Symposium on Mathematical and Computational Oncology* (ISMCO'20). Virtual. October 2020.
- Program Committee Member for the *Second International Symposium on Mathematical and Computational Oncology* (ISMCO'20). Virtual. October 2020.
- 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

- *Journal for ImmunoTherapy of Cancer*, SITC & BMJ. 2025 – to date.
- *Cancer Informatics*, SAGE. 2025 – to date.
- *NAR Genomics and Bioinformatics*, Oxford. 2025 – to date.
- *Advanced Science*, Wiley. 2025 – to date.
- *Scientific Data*, Nature. 2024 – to date.
- *Scientific Reports*, Nature. 2024 – to date.
- *Cancer Immunology, Immunotherapy*, Springer. 2024 – to date.
- *BMC Bioinformatics*, Springer Nature. 2023 – to date.

- *Nature Communications*, Nature. 2023 – to date.
- *Protein Science*, Wiley. 2023 – to date.
- *Viruses*, Multidisciplinary Digital Publishing Institute (MDPI). 2022 – to date.
- *PLoS Computational Biology*, PLoS Journals. 2021 – to date.
- *Frontiers in Molecular Biosciences*, Frontiers Journals. 2020 – to date.
- *ACS Nano*, American Chemical Society (ACS) Publications. 2020 – to date.
- *Computer Physics Communications*, Elsevier. 2020 – to date.
- *BMC Molecular and Cell Biology*, Springer Nature. 2020 – to date.
- *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

- NIH study section: Special Emphasis Panel (SEP). October 2025.
- NIH study section: Basic Cancer Immunobiology (BCIB). March 2025.
- 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.

ADVISING OF STUDENTS

Trainees for whom I served as primary mentor

Trainee name	Level	UH Program	Institution	Period
Yasmina Rezai	undergrad. std.	-	U. of Houston	2024 – to date
Julia F. P. De Almeida	undergrad. std.	-	U. of Houston	2024 – 2025
Gabriel Gavez	undergrad. std.	-	U. of Houston	2024 – 2025
Victoria J. Huang	high-school std.	-	U. of Houston	2024 – 2025
Hangqing Lin	rotation grad. std.	BCHS	U. of Houston	2024
Oscar Olbera	undergrad. std.	-	U. of Houston	2024 – 2025
Anderson J. Castilla Sedano	rotation grad. std.	BCHS	U. of Houston	2023
Alfredo Calderón-Macedo	undergrad. std.	-	U. of Houston	2023 – to date
Uyen Do	undergrad. std.	-	U. of Houston	2023 – to date
Akash Borigi	grad. std.	MSEDS	U. of Houston	2023 – 2024
Martiela Vaz de Freitas	Postdoc. Fellow	-	U. of Houston	2022 – 2025
Pamela Borges	grad. std.	CMB	U. of Houston	2022 – to date
Finn Beruldsen	grad. std.	BCHS	U. of Houston	2022 – to date
San Tran	undergrad. std.	-	U. of Houston	2022 – 2023
↪	rotation grad. std.	BCHS	U. of Houston	2024
Hoa Nhu Le	grad. std.	CMB	U. of Houston	2021 – 2024
Jaila D Lewis	grad. std.	BCHS	U. of Houston	2021 – to date
Sae Hee E Choi	grad. std.	CMB	U. of Houston	2021 – to date
André Fonseca	Postdoc. Fellow	-	U. of Houston	2021 – 2022
Hussain Kalavadwala	rotation grad. std.	CMB	U. of Houston	2021 – 2022
Alexandra Bishop	undergrad. std.	-	Rice U.	2019
Karen Wong	undergrad. std.	-	Rice U.	2015
Sujey Tadwalker	undergrad. std.	-	Rice U.	2015

Trainees for whom I served as secondary mentor or co-mentor

Trainee name	Level	UH Program	Institution	Period
Francisca Joseli de Souza	grad. std.	-	UFC (Brazil)	2023 – to date
Cinthia Alves	Postdoc. Fellow	-	USP (Brazil)	2021 – to date
Seungheon (Kevin) Lee	grad. std.	-	U. of Houston	2021 – 2022
Anja Conev	grad. std.	-	Rice U.	2019 – to date
Romanos Fasoulis	grad. std.	-	Rice U.	2019 – to date
Sarah Hall-Swan	grad. std.	-	Rice U.	2018 – to date
Kyle R. Jackson	grad. std.	-	UT MD Anderson	2016 – 2020
Jayvee R. Abella	grad. std.	-	Rice U.	2015 – 2019
Marcus F. A. Mendes	grad. std.	-	UFRGS (Brazil)	2012 – 2014
Marcelo Bragatte	undergrad. std.	-	UFRGS (Brazil)	2013 – 2014
Martiela Freitas	undergrad. std.	-	UFRGS (Brazil)	2013 – 2014
Renata F. Tarabini	undergrad. std.	-	UFRGS (Brazil)	2013 – 2014
Caio Diniz	undergrad. std.	-	UFRGS (Brazil)	2013
Tahila Andrighetti	undergrad. std.	-	UFRGS (Brazil)	2013
Francis Maria Báo Zambra	grad. std.	-	UFRGS (Brazil)	2011 – 2012
Jader P. da Silva	undergrad. std.	-	UFRGS (Brazil)	2011 – 2012
Daniele F. Figueiredo	grad. std.	-	UFRGS (Brazil)	2010 – 2012
Cassiana C. Fülber	undergrad. std.	-	UFRGS (Brazil)	2009 – 2010
Bruna Correa	undergrad. std.	-	UFRGS (Brazil)	2009

University of Houston Graduate Program Codes:
BCHS, PhD in Biochemistry; Bio. & Biochem. Dept., NSM
CMB, PhD in Biology, Cell and Molecular Biology Track; Bio. & Biochem. Dept., College of Natural Sciences and Mathematics.
MSEDS, Master of Science in Engineering Data Science; Cullen College of Engineering

LECTURES, TUTORIALS AND INVITED TALKS

Since 2017, I have organized and presented several short courses and tutorials on bioinformatics methods and their applications to immunology, vaccinology and cancer immunotherapy. I have also presented a number of invited talks and lectures in topics related to my research (more at my dinlerantunes.com).
My next and most recent talks (2024-2025) include:

- *AI-based structural modeling of TCR and their targets: Advances and Limitations.* Invited talk at the "Leveraging the Power of Artificial Intelligence to Foster Progress in Immuno-oncology: Opportunities and Challenges", a Pre-Conference event of the 40th Anniversary SITC symposium.
National Harbor, MD, US. November 6, 2025.
- *Computational biology applied to drug discovery and cancer immunotherapy.* Invited talk at *Universidade do Vale do Taquari (Univates)*, as part of the course on Advanced Topics in Medicine and Health Science. Lajeado, RS, Brazil (via Zoom). August 21, 2025.
- *HLA-Arena: Integrating structural bioinformatics on the design of personalized immunotherapies.* Invited talk at the Postgraduate Program in Genetics and Molecular Biology of the Federal University of Rio Grande do Sul (PPGBM/UFRG). Porto Alegre, RS, Brazil. August 14, 2025.
- *Artificial intelligence powered biomedical research.* Invited talk at the The Advanced Technology and Medical Research Exploration, a Biomedical Research Incubator program by the Center for Nuclear Receptors of the University of Houston, and the Lester and Sue Smith Breast Center of the Baylor College of Medicine. Houston, TX, US. July 15, 2025.
- *HLA-Arena: Enabling structure-guided pipelines for personalized cancer immunotherapy design.* Invited talk at the NCI intramural webinar series, for the Computational Genomics and Bioinformatics Branch (CGBB) of the NCI's Center for Biomedical Informatics and Information Technology (CBIIT). Bethesda, MD, US (via Webex; recording). April 30, 2025.
- *ML-based consensus scoring for optimized peptide-ligand virtual screening.* Invited talk at the Drug Discovery Institute (DDI) of the University of Houston. Houston, TX, US. April 7, 2025.
- *AI and structural bioinformatics methods for drug discovery.* Lecture in class "Drug Design and Discovery" (PCOL6345). Course offered to Graduate students from the College of Pharmacy at the University of Houston. Houston, TX, US. April 2-4, 2025.
- *Improving the Design of Immunotherapies.* Invited talk for the Innovative Research Talk series of the HEALTH Center for Addictions Research and Cancer Prevention (HEALTH-RCMI). Houston (via Zoom), TX, US. March 20, 2025.
- *AI and structural bioinformatics methods for drug discovery.* Lecture in class "Technologies for Cancer Drug Discovery & Development" (GS-CC-6401). Course offered to Graduate students from both Baylor College of Medicine (BCM) and the University of Houston. Houston, TX, US. March 28, 2025.
- *Improving the design of immunotherapies for underrepresented minorities.* Invited talk at the meeting of the Community Research Advisory Board (CRAB), in partnership with the HEALTH Center for Addictions Research and Cancer Prevention (HEALTH-RCMI). Houston (via Zoom), TX, US. March 4, 2025.
- *Novel cancer immunoinformatics pipelines to advance personalized T-cell-based immunotherapies.* Invited talk at the GCC's Keck Seminar. Houston, TX, US. November 15, 2024.
- *Improving the design of immunotherapies for underrepresented minorities.* Invited talk at the meeting of the Community Research Advisory Board (CRAB), in partnership with the HEALTH Center for Addictions Research and Cancer Prevention (HEALTH-RCMI). Houston (via Zoom), TX, US. May 7, 2024.
- *From Gauchos to Cowboys: My academic path to the University of Houston.* Invited talk at the Seminars of the Post-Graduate Program in Cellular and Molecular Biology (PPGBCM), at the Biotechnology Center of the Federal

University of Rio Grande do Sul (CBiot/UFRGS/Brazil). Porto Alegre (via Zoom), RS, Brazil. April 26, 2024.

- *Structural Modeling and Dynamic Contact Analysis of TCRpHLA Complexes.* Invited talk at "GCC 4th Annual Future of Immunology Symposium" (IMM24), by GCC Immunology Consortium. Houston, TX, US. April 9, 2024.
- *AI and structural bioinformatics methods for drug discovery.* Lecture in class "Technologies for Cancer Drug Discovery & Development" (GS-CC-6401). Course offered to Graduate students from both Baylor College of Medicine (BCM) and the University of Houston. Houston, TX, US. February 2nd, 2024.

Hands-on Tutorials/Workshops

- *Bioinformatics and Cancer Treatment Lab.* Scheduled hands-on workshop for high-shool students of the 3rd and 5th Wards in Houston, being organized in partnership with the HEALTH Center for Addictions Research and Cancer Prevention (HEALTH-RCMI). Houston, TX, US. Planned for January 2026.
- *Novel computational approaches for immunotherapy design.* Hands-on workshop for graduate students of the Postgraduate Program in Molecular and Cell Biology at the Federal University of Rio Grande do Sul (PPGBCM/UFRGS). Porto Alegre, RS, Brazil. Duration: 3 hours. May 2025
- *iTECH-STEM.* Hands-on Biotechnology Summer Camp on protein visualization, molecular docking and virtual screening, ministered to both graduate and undergraduate students at the Science and Engineering Research Center of University of Houston. Houston. Duration: 4 weeks. June 2023.
- *iTECH-STEM.* Hands-on Biotechnology Summer Camp on protein visualization, molecular docking and virtual screening, ministered to both graduate and undergraduate students at the Science and Engineering Research Center of University of Houston. Houston. Duration: 2 weeks. June 2022.
- *Current methods and open challenges for structural modeling in cancer immunotherapy (2nd Ed.).* Tutorial held as part of the Second International Symposium on Mathematical and Computational Oncology (ISMCO'20). Virtual. Duration: 4 h. 2020
- *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
- *Bionformatics 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
- *Bionformatics 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
- *Bionformatics 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

RELEVANT INTERVIEWS AND NEWS ARTICLES

Personalized Cancer Treatment: UH Research Team Awarded R21 Grant to Improve Safety of Immunotherapy,
by Alison Medley at NSM News and Events.

UH Researchers Strive to Improve Cancer Treatment for Minority Patients,
by Brooke Lewis at City Cast Houston.

UH Research Team Awarded Pilot Program Grant from HEALTH-RCMI,
by Alison Medley at NSM News and Events.

Making immunotherapy safer,
by Laurie Fickman at UH Newsroom.

Dr. Dinler Antunes: Cancer immunotherapy,
by Leo Elworth for "The Bioinformatics and Beyond Podcast".

Dr. Dinler Antunes: Protein Folding, AlphaFold2, Molecular Docking,
by Leo Elworth for "The Bioinformatics and Beyond Podcast".

OTHER SKILLS

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 LaTeX, 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.