DINLER A. ANTUNES, DSc

EMAIL: dinler@uh.edu **HOMEPAGE:** dinlerantunes.com
OFFICE: Science and Engineering Research Center (SERC), Suite 3007.
3517 Cullen Blvd, Bldg. 545, Houston, TX 77204-5056

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:
$\ast$, shared first autorship.
$\propto$, 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.

57. Borges P†, Vaz de Freitas M‡, Yoo J, Beruldsen F†, Lewis J†, Freitas de Sousa FJ†, Choi SH†, Nguyen DB, Zanatta G, Jang JH, Donadi E, Alachkar H, Wolf S, Rigo M, Jeon H, and Antunes DA$^{\propto}$. Mapping the TCR landscape: computational tools empowering translational immunology and therapy design. *J Immunother Cancer*, 14(6):e014184, 2026 (link).

56. Trujillo-Ocampo A, Borges P†, Grefe M, Vaz de Freitas M‡, Lee SE, Qi Y, Clinton J, Li D, He H, Yu L, Peris-Cuesta A, Ehli E, Ma Q, Su X, Antunes DA, Alatrash G, Molldrem JJ, Shpall E, and Im JS$^{\propto}$. Human NKT10 cells are enriched in cord-derived invariant Natural Killer T cells and mediate immune-regulation in a xenogeneic graft-versus-host disease model. *Front Immunol*, 2026. manuscript accepted for publication

55. Beruldsen F†, Vaz de Freitas M‡, and Antunes DA$^{\propto}$. High resolution mapping of protein motions in time and space with RMSX and Flipbook. *Scientific Reports*, 16(1):10035, 2026 (link).

54. Dasdemir E, Veletic I, Ly CP, Quesada AE, Pacheco CD, Jelloul FZ, Borges P†, Basu S, Jindal S, Wang Z, Lazar A, Wani KM, Antunes DA, Reville PK, Gunaratne PH, Tower RJ, Sharma P, and Abbas H$^{\propto}$. Integrative spatial multi-omics reveal niche-specific inflammatory signaling and differentiation hierarchies in acute myeloid leukemia. *iScience*, November 2025

53. de Sousa FJF†, Antunes DA$^{\propto}$, and Zanatta G$^{\propto}$. PI3K-Seeker: A Machine Learning-Powered Web Tool to Discover PI3K Inhibitors. *ACS Omega*, November 2025 (pdf).

52. Castillo MB, Rankothgedera S, Thevasagayampillai S, Kandasamy A, Lewis J†, Woody C, Vaz de Freitas M‡, Antunes DA, El-Zein R, and Gunaratne PH$^{\propto}$. Identification of immunogenic KIF5B-RET fusion neopeptides driving immune stimulation in tumor specific CD8+ T cells. *Frontiers in immunology*, 16:1635810, 2025 (link).

51. Arman P, Haghighijoo Z, Lupascu CA, Singh AK, Goode NA, Baumgartner TT, Singh J, Xue Y, Wang P, Chen H, Antunes DA, Lijffijt M, Zhou J, Migliore M, and Laezza F$^{\propto}$. FGF14 Peptide Derivative Differentially Regulates Nav1.2 and Na(v)1.6 Function. *Life (Basel, Switzerland)*, 15(9), August 2025 (link).

50. Alves CC, Lewis J†, Antunes DA$^{\propto}$, and Donadi EA$^{\propto}$. 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. Le HN†, Vaz de Freitas M‡, and Antunes DA$^{\propto}$. Strengths and limitations of web servers for the modeling of TCRpMHC complexes. *Comput Struct Biotechnol J*, 23, July 2024 (pdf).

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

47. Fasoulis R, Rigo MM, Lizée G, Antunes DA, and Kavraki LE[∝]. 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. Antunes DA[∝], Baker BM, Cornberg M, and Selin LK. Quantification and prediction of t-cell cross-reactivity through experimental and computational methods. *Front Immunol*, 15, Feb 2024 (link).

45. Antunes DA[∝], Schoeder CT, Minkyung B, and Donadi EA. Editorial: Structural modeling and computational analyses of immune system molecules. *Front Immunol*, 15, Feb 2023 (link).

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

43. Fasoulis R, Rigo MM, Antunes DA, Paliouras G[∝], and Kavraki LE[∝]. Transfer learning improves pMHC kinetic stability and immunogenicity predictions. *Immunoinformatics.*, 13, Dec 2023 (link).

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

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

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

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

38. Desai P, Wang B, Fonseca AF[‡], Borges P[†], Jelloul F, Reville P, Lee E, Ly C, Basi A, Root J, Baran N, Post S, Deng Q, Sun H, Harmanci A, Burks J, Gomez J, DiNardo C, Daver N, Al-Atrash G, Konopleva M, Green M, Antunes DA, Hao FD, and Abbas H[∝]. 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. Sonnemann HM, Pazdrak B, Antunes DA, Roszik J, and Lizée G[∝]. 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. Lee SE, Wang F, Grefe M, Trujillo-Ocampo A, Ruiz-Vasquez W, Takahashi K, Abbas HA, Borges P[†], Antunes DA, Al-Atrash G, Daver N, Molldrem JJ, Futreal A, Garcia-Manero G, and Im JS[∝]. Immunologic Predictors for Clinical Responses during Immune Checkpoint Blockade in Patients with Myelodysplastic Syndromes. *Clin Cancer Res*, pages OF1–OF14, Mar 2023 (link).

35. Alves CC, Arns T, Oliveira ML, Moreau P, Antunes DA, Castelli EC, Mendes-Junior CT, Giuliatti S, and Donadi EA[∝]. 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. Jackson KR*, Antunes DA*, Talukder AH, Maleki AR, Amagai K, Salmon A, Katailiha AS, Chiu Y, Fasoulis R, Rigo MM, Abella JR, Melendez BD, Li F, Sun Y, Sonnemann HM, Belousov V, Frenkel F, Justesen S, Makaju A, Liu Y, Horn D, Lopez-Ferrer D, Huhmer AF, Hwu P, Roszik J, Hawke D, Kavraki LE, and Lizée G$^{\propto}$. 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. Rigo MM, Fasoulis R, Conev A, Hall-Swan S, Antunes DA$^{\propto}$, and Kavraki LE$^{\propto}$. 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. Conev A, Devaurs D, Rigo MM, Antunes DA$^{\propto}$, and Kavraki LE$^{\propto}$. 3pHLA-score improves structure-based peptide-HLA binding affinity prediction. *Sci Rep*, 12(1):10749, Jun 2022 (pdf).

31. Sapoval N, Aghazadeh A, Nute MG, Antunes DA, Balaji A, Baraniuk R, Barberan CJ, Dannenfelser R, Dun C, Edrisi M, Elworth RAL, Kille B, Kyrillidis A, Nakhleh L, Wolfe CR, Yan Z, Yao V, and Treangen TJ$^{\propto}$. Current progress and open challenges for applying deep learning across the biosciences. *Nat Commun*, 13(1):1728, Apr 2022 (pdf).

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

29. Tarabini RF, Rigo MM, Fonseca AF‡, Rubin F, Bellé R, Kavraki LE, Ferreto TC, Antunes DA$^{\propto}$, and de Souza APD$^{\propto}$. 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. Hall-Swan S, Devaurs D, Rigo MM, Antunes DA$^{\propto}$, Kavraki LE$^{\propto}$, and Zanatta G$^{\propto}$. DINC-COVID: A webserver for ensemble docking with flexible SARS-CoV-2 proteins. *Comput Biol Med*, 139:104943, Dec 2021 (pdf).

27. Abella JR, Antunes DA, Jackson K, Lizée G, Clementi C, and Kavraki LE$^{\propto}$. 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. Arns T, Antunes DA, Abella JR, Rigo MM, Kavraki LE, Giuliatti S, and Donadi EA$^{\propto}$. Structural modeling and molecular dynamics of the immune checkpoint molecule HLA-G. *Frontiers in Immunology*, 11:2882, Nov 2020 (pdf).

25. Antunes DA, Abella JR, Hall-Swan S, Devaurs D, Conev A, Moll M, Lizée G, and Kavraki LE$^{\propto}$. 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. Devaurs D, Antunes DA, and Kavraki LE$^{\propto}$. Computational analysis of complement inhibitor compstatin using molecular dynamics. *J. Mol. Model.*, 26(9):231, Aug 2020 (pdf).

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

22. Soon CF, Zhang S, Suneetha PV, Antunes DA, Manns MP, Raha S, Schultze-Florey C, Prinz I, Wedemeyer H, Sallberg Chen M, and Cornberg M$^{\propto}$. Hepatitis E Virus (HEV)-Specific T Cell Receptor Cross-Recognition: Implications for Immunotherapy. *Front. Immunol.*, 10:2076, Sep 2019 (pdf).

21. Devaurs D, Antunes DA, Hall-Swan S, Mitchell N, Moll M, Lizée G, and Kavraki LE$^{\propto}$. 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. Abella JR, Antunes DA, Clementi C, and Kavraki LE$^{\propto}$. APE-Gen: A fast method for generating ensembles of bound peptide-MHC conformations. *Molecules*, 24(5):881, Mar 2019 (pdf).

19. Antunes DA, Abella JR, Devaurs D, Rigo MM, and Kavraki LE$^{\propto}$. 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. Devaurs D, Antunes DA, and Kavraki LE$^{\propto}$. Revealing unknown protein structures using computational conformational sampling guided by experimental hydrogen-exchange data. *Int. J. Mol. Sci.*, 19(11):3406, 2018 (pdf).

17. Antunes DA, Devaurs D, Moll M, Lizée G, and Kavraki LE$^{\propto}$. General Prediction of Peptide-MHC Binding Modes Using Incremental Docking: A Proof of Concept. *Sci. Rep.*, 8(1):4327, Mar 2018 (pdf).

16. Antunes DA, Rigo MM, Freitas MV, Mendes MFA, Sinigaglia M, Lizée G, Kavraki LE, Selin LK, Cornberg M, and Vieira GF$^{\propto}$. Interpreting T-cell cross-reactivity through structure: Implications for TCR-based cancer immunotherapy. *Front. Immunol.*, 8:1210, 2017 (pdf).

15. Antunes DA, Moll M, Devaurs D, Jackson KR, Lizée G, and Kavraki LE$^{\propto}$. DINC 2.0: A New Protein-Peptide Docking Webserver Using an Incremental Approach. *Cancer Res.*, 77(21):e55–e57, Nov 2017 (pdf).

14. Devaurs D, Antunes DA, Papanastasiou M, Moll M, Ricklin D, Lambris JD, and Kavraki LE$^{\propto}$. Coarse-Grained Conformational Sampling of Protein Structure Improves the Fit to Experimental Hydrogen-Exchange Data. *Front. Mol. Biosci.*, 4:13, 2017

13. Devaurs D, Papanastasiou M, Antunes DA, Abella JR, Moll M, Ricklin D, Lambris JD, and Kavraki LE$^{\propto}$. 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. Mendes MF*, Antunes DA*, Rigo MM, Sinigaglia M, and Vieira GF$^{\propto}$. Improved structural method for T-cell cross-reactivity prediction. *Mol. Immunol.*, 67(2 Pt B):303–310, Oct 2015

11. Antunes DA, Devaurs D, and Kavraki LE$^{\propto}$. Understanding the challenges of protein flexibility in drug design. *Expert Opin. Drug. Discov.*, 10(12):1301–1313, Dec 2015

10. Rigo MM, Antunes DA, Vaz de Freitas M, Fabiano de Almeida Mendes M, Meira L, Sinigaglia M, and Vieira GF$^{\propto}$. DockTope: a Web-based tool for automated pMHC-I modelling. *Sci. Rep.*, 5:18413, Dec 2015

9. Zhang S, Bakshi RK, Suneetha PV, Fytili P, Antunes DA, Vieira GF, Jacobs R, Klade CS, Manns MP, Kraft AR, Wedemeyer H, Schlaphoff V, and Cornberg M$^{\propto}$. 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. Figueiredo DF*, Antunes DA*, Rigo MM, Mendes MF, Silva JP, Mayer FQ, Matte U, Giugliani R, Vieira GF, and Sinigaglia M$^{\propto}$. Lessons from molecular modeling human α-L-iduronidase. *J. Mol. Graph. Model.*, 54:107–113, Nov 2014

7. Antunes DA, Rigo MM, Sinigaglia M, de Medeiros RM, Junqueira DM, Almeida SE, and Vieira GF$^{\propto}$. New insights into the in silico prediction of HIV protease resistance to nelfinavir. *PLoS ONE*, 9(1):e87520, 2014

6. Sinigaglia M, Antunes DA, Rigo MM, Chies JA, and Vieira GF$^{\propto}$. CrossTope: a curate repository

of 3D structures of immunogenic peptide:MHC complexes. *Database (Oxford)*, 2013:bat002, 2013

5. Rigo MM, Antunes DA, Cibulski SP, Sinigaglia M, Chies JA, and Vieira GF$^{\propto}$. Immunogenic epitopes of Hantaviruses' N protein are restricted to conserved regions. *Front. Biosci. (Landmark)*, 17:1582–1588, Jan 2012

4. Campos FS, Dezen D, Antunes DA, Santos HF, Arantes TS, Cenci A, Gomes F, Lima FE, Brito WM, Filho HC, Batista HB, Spilki FR, Franco AC, Rijsewijk FA, and Roehe PM$^{\propto}$. Efficacy of an inactivated, recombinant bovine herpesvirus type 5 (BoHV-5) vaccine. *Vet. Microbiol.*, 148(1):18–26, Feb 2011

3. Varela AP, Holz CL, Cibulski SP, Teixeira TF, Antunes DA, Franco AC, Roehe LR, Oliveira MT, Campos FS, Dezen D, Cenci A, Brito WD, and Roehe PM$^{\propto}$. 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. Antunes DA, Rigo MM, Silva JP, Cibulski SP, Sinigaglia M, Chies JA, and Vieira GF$^{\propto}$. 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. Antunes DA*, Vieira GF*, Rigo MM, Cibulski SP, Sinigaglia M, and Chies JA$^{\propto}$. 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

Theses

3. Antunes DA. *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. Antunes DA. *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. Antunes DA. *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).

AWARDS AND HONORS BY ANTUNES LAB TRAINEES

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.

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
2026	James P. Taylor Foundation Scholarship for GCC2026 (Clermont-Ferrand, France)	Finn Beruldsen
2026	Best Poster Award at 30th Structural Biology Annual Symposium (UTMB, Galveston)	Jaila Lewis
2026	Best Oral Presentation Bioscience Graduate Society Symposium (UH, Houston)	Jaila Lewis
2025	Travel Award for the NIH/NCI's ITCR Annual Meeting (Rockville, Maryland)	Finn Beruldsen
2025	NSM Graduate Conference Travel Fellowship from the NSM College (UH, Houston)	Finn Beruldsen
2025	Student Travel Award from the Department of Biology and Biochemistry (UH, Houston)	Finn Beruldsen
2025	Distinguished Graduate Student Leadership Award (UH, Houston)	Finn Beruldsen
2025	Cullen Fellowship Travel Grant from the UH's Graduate School (UH, Houston)	Jaila Lewis
2025	Student Travel Award Department of Biology and Biochemistry (UH, Houston)	Jaila Lewis
2025	Excellence in Mentorship Award from the Bioscience Graduate Society (UH, Houston)	Jaila Lewis
2023	Best Poster award at 27th Structural Biology Annual Symposium (UTMB, Galveston)	Jaila 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)	Jaila Lewis
2022	University of Houston Presidential Fellowship (UH, Houston)	Finn Beruldsen
2021	Best Poster award at CNRCS Annual Research Symposium (UH, Houston)	André Fonseca

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.

OTHER EXPERIENCE AND PROFESSIONAL MEMBERSHIPS

- Member of the NCI's Cancer Immunoprevention Network (CIP-Net), 2026 – to date
- 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.

LECTURES, TUTORIALS AND INVITED TALKS

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.