

Jaila D. Lewis, B.S.

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Personal Statement

I am a 5th year Ph.D. Candidate in the Biochemistry Division at the University of Houston. I specialize in structural bioinformatics and immunoinformatics techniques to improve the design of cancer immunotherapies and viral vaccines. I am developing immunoinformatic pipelines that aim to provide safe and efficacious cancer vaccine candidates and achieve equitable healthcare for all. My ultimate career goal is to provide high-quality immunotherapies for cancer and autoimmune diseases for all patients, especially understudied patients of color.

Education

Ph.D. in Biochemistry

University of Houston, Houston, Texas. Degree expected in May 2026.

B.S. in Biochemistry and Molecular Biology

Minors: Biology, Chemistry, Philosophy, and Religion

Mercer University, Macon, Georgia. Degree earned May 2021.

Research Projects

Improving the Design of Immunotherapies for Understudied Patients of Color: Thesis Project

Principle Investigator: Dr. Dinler Antunes December 2022 – Present

Cancer immunotherapy leverages a patient's immune system, enabling the required immunological responses and memory to combat diseases like cancer or infections. However, this innovative treatment is not accessible for all. Due to many limitations impacting the healthcare system (e.g., lack of representation in clinical trials), understudied patients of color (UPCs) may not receive the benefits of immunotherapy. Instead, they can experience higher rates of toxicity and death when treated with some cancer immunotherapies. Therefore, it is imperative we address this health inequity with inclusive treatment design. In my thesis, I combine sequence-based algorithms and structural modeling to identify high-quality and generalized peptide cancer vaccine candidates for UPCs. I developed a new tool, PPmGen, to design highly biochemically similar, altered peptide ligands for the human leukocyte antigen (HLA) alleles restricted to UPCs. As a result, I yielded 90 peptide candidates that are safer, more efficacious, and generalized for all the UPC alleles of interest. These findings are currently being experimentally validated. This project was funded under the National Institute on Minority Health and Health Disparities (NIMHD) of the National Institutes of Health (NIH) to the University of Houston under Award Number U54MD015946.

Discovery of Immunogenic Neopeptides from Actionable Chimeric RNAs to Develop Vaccines for Lung and Breast Cancer Treatment

Principle Investigators: Dr. Dinler Antunes and Dr. Preethi Gunaratne June 2023 - Present

Cancer is a worldwide problem, altering the lives of many. Somatic mutations in key genes can cause multiple diseases, including different types of cancer. One somatic mutation event is known as gene fusions, where two chromosomes can recombine, translocate, or experience deletions with each other, giving rise to multiple different cancer types, like breast or lung cancer. In collaboration with the Gunaratne Lab at UH and MD Anderson, we identified fusion neoantigens expressed by patients diagnosed with non-small-cell lung cancer and breast cancer and tested their ability to be used in a cancer vaccine. I utilized molecular docking with our tool APE-Gen2.0 to predict the binding of fusion neoantigens from lung and breast cancer to the human leukocyte antigen (HLA) receptors expressed by the patients. I also predicted the risk of off-target toxicity associated with T-cell cross reactivity for the fusion neopeptides. Our predictions were validated by wet lab techniques like ELISpot. We have completed both these projects, published the work for the *KIF5B-RET* lung cancer project, and aim to publish our findings from the breast cancer project.

Analyzing Dynamic Interactions of Drug Activators for the Pseudokinase MLKL

Principle Investigators: Dr. Dinler Antunes and Dr. Greg Cuny August 2022 – August 2024

Innate immunity hosts essential immune processes against cancer and viral infections. A particular mechanism is the necroptosis pathway, regulates inflammatory cell death towards diseased cells. Certain tumors, however, can downregulate necroptosis. These are called *cold* tumors (i.e., tumors unresponsive to immunotherapy) and are associated with particular cancers. Therefore, identifying ligands capable of directly triggering necroptosis in *cold* tumors represents a promising avenue for treatment. Our team identified small molecule activators to target and activate mixed lineage kinase domain (MLKL) pseudokinase, which is a downstream executioner in the necroptosis pathway and may be a promising avenue for increasing antitumor activity against *cold* tumors. We paired *in vitro* experiments to observe the activation of necroptosis with molecular docking and molecular dynamics simulations to analyze the structure-activity relationship for ligand binding to both the open inactive and closed active conformations of MLKL. If successful, we will elucidate the interactions required for activating MLKL, guide our *in vitro* experiments, and provide direct applications for targeting *cold* tumors. This project was funded by UH's Drug Discovery Institute (DDI).

Evaluation of Scoring Functions to Rank Bound Conformations of Peptide-HLA Complexes

Principle Investigator: Dr. Dinler Antunes October 2021 – Present

Cancer immunotherapies are very promising, however; they experience limitations, especially regarding the genetic diversity of different patients and cancers. One contribution of these experienced limitations could be the use of the gold-standard human leukocyte antigen (HLA) binding algorithms. These sequence-based algorithms are trained on large datasets from databases like The Cancer Genome Atlas (TCGA), which has an underrepresentation of non-White patients. This data bias can cause an algorithmic bias, which might yield inaccurate HLA binding predictions for HLA alleles prevalently found in understudied patients. Instead, we proposed that structure-based methods (e.g., molecular docking) can better categorize peptide binders and conformations for many diverse HLA receptors, not just the alleles most commonly studied. I used our meta-docking tool DINC (Docking INCrementally) to predict the structure of the validated crystallized peptide-HLA complexes to yield multiple conformations with ranging Root Mean Square Deviations (RMSD) values, with the lowest RMSD values representing the best structures. However, structure-based methods are limited in determining the best or biologically feasible peptide-HLA conformations. Therefore, we evaluated 11 alternate SFs in their rankings of the several peptide-HLA conformations per crystal structure. We concluded we should combine these diverse SFs in a consensus method to develop an accurate, user-friendly scoring function for protein-ligand complexes, especially for peptide-HLA complexes. We worked alongside Rice University, UH-Downtown, UH, and immunologists from the MD Anderson Cancer. We expanded this project to develop an AI and structure-based SF, which was funded by UH's Drug Discovery Institute.

Publications

Castillo MB, Rankothgedera S, Thevasagayampillai S, Kandasamy A, Lewis J, Woody C, Vaz de Freitas M, Antunes DA, El-Zein R and Gunaratne PH (2025) Identification of immunogenic KIF5B-RET fusion neopeptides driving immune stimulation in tumor specific CD8+ T cells. *Front. Immunol.* 16:1635810. doi: 10.3389/fimmu.2025.1635810

Alves CC, Lewis J, Antunes DA, Donadi EA. The Role of Vimentin Peptide Citrullination in the Structure and Dynamics of HLA-DRB1 Rheumatoid Arthritis Risk-Associated Alleles. *Int J Mol Sci.* 2024 Dec 24;26(1):34. doi: 10.3390/ijms26010034. PMID: 39795892; PMCID: PMC11719467.

Awards and Grants

Department of Biology and Biochemistry First Annual Gala - **Excellence in Mentorship Award, May 2025**

National Institute of Minority Health and Health Disparities R01 Grant – **Assisted in writing the application, May 2025, application selected for review**

University of Houston's Helping Everyone Achieve a Lifetime of Health (HEALTH) Center for Addictions Research and Cancer Prevention Pilot Grant Program – **Funding approved March 2024**

SACNAS National Diversity in STEM Conference, October 2023, Portland, Oregon – **Best Poster Award**

Sealy Center for Structural Biology Symposium, April 2023 University of Texas Medical Branch, Galveston, Texas – **Best Poster Award**

University of Houston Drug Discovery Institute – **Funding Approved April 2023**

Center of Nuclear Receptor and Cellular Signaling Symposium, University of Houston, December 2022, Houston, Texas – **Best Poster Award**