Aldo HERRERA RODULFO

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Professional Summary

Biomolecular research scientist with a strong interest and expertise in computational methods for biological systems. Passionate about uncovering biomolecular mechanisms at the molecular level through physics- and AI-driven computational approaches. Experienced in molecular biophysics and in the development of bioinformatics tools to drive innovation and advance biomedical and biotechnological research.

Education

Center for Research and Advanced Studies of the IPN, Monterrey Unit (CINVESTAV)
PhD in Biomedical Engineering and Physics | 2020 - 2025*
Thesis: ***The Role of Conformational Dynamics Conservation in the Structure-Function Paradigm: A Case Study on the RBD of SARS-CoV-2 Spike Protein Variants.***

Stay Abroad Saarbrücken, Germany
Helmholtz Institute for Pharmaceutical Research Saarland (HIPS) | May-August 2023
Project: ***Designing a computational framework for protein-ligand interaction analysis using modern artificial intelligence architectures and graph theory.***

Autonomous University of Nuevo León (UANL)
Master's in Science with a focus on Pharmacy | 2018-2020
Thesis: ***Analysis of N-acetyltransferase 2 (NAT2) gene polymorphisms as markers of liver damage from first-line tuberculosis treatment in a population from northeastern Mexico, and molecular dynamics studies.***

Autonomous University of Nuevo León (UANL)
Pharmaceutical Biologist Chemist | 2013-2018

Skills & Expertise

Technical: Python, R, Bash, Nextflow, GROMACS, RDKit, Pandas, Matplotlib, Seaborn, NumPy, SciPy, Scikit-learn, PyTorch, TensorFlow, AutoDock, Vina, CHARMM, AMBER, NAMD, OpenMM, PyMOL, Chimera, Biopython, MDAnalysis, PLIP, PyRosetta, Git, Docker, Slurm, HPC Environments, Linux/Unix Systems, Data Visualization, Machine Learning for Molecular Modeling, High-Throughput Virtual Screening, Free Energy Calculations, Molecular Docking, PCA Analysis, Hydrogen Bond Analysis, Conformational Entropy Analysis. **Laboratory:** Micropipette, Solution Preparation, Centrifugation, UV-Vis Spectrophotometry, Titration, Bacterial Culture, Gram Staining, Autoclaving, PCR. **Soft skills:** Self-motivated, curious, creative, team player, solution-focused, willing to learn, willing to listen, willing to acquire new technical skills, supportive, critical thinker, punctual, proactive, adaptable, detail-oriented, resourceful, resilient, independent, organized, empathetic, collaborative, and results-driven. **Languages:** Spanish (Native), English Conversational (C2, certified): EFSET Certificate**.**

Coding portfolio [github: https://github.com/aldhr]:
Drug-target interaction miner: Extracts protein-ligand information from PDB IDs into graph format for Graph Neural Network input. GitFront
Bash-Scripting Pipeline: Automates multiple-cycle molecular docking analysis, processes files into AutoDock VINA inputs, formats output into CSV for further analysis**.** GitFront
Cheminformatics Analysis Notebooks: Analyzes distribution of molecular docking sets, visualizes protein frequent electrostatic interactions**.** GitFront
Colab notebooks: Protein-DNA docking using PyDock DNA (here) & Protein-Ligand molecular dynamics simulations (here).

Publications

2025

[Research article, **First Author**] **Herrera-Rodulfo, A**., Andrade-Medina, M., García-Delgado, M.S., & Carrillo-Tripp, M. (In Press, 2025). **Extensive In-silico Target-Ligand Conformational Space Sampling of Garlic-Derived Sulfur Compounds targeting COVID-19 infection.** *Journal of Computational Biophysics and Chemistry*.

[Research article, Co-**Author**]
Granados-Tristán, A. L., Carrillo-Tripp, M., Hernández-Luna, C. E., **Herrera-Rodulfo, A.**, González-Escalante, L. A., Arriaga-Guerrero, A. L., Silva-Ramírez, B., Escobedo-Guajardo, B. L., Mercado-Hernández, R., Bermúdez de León, M., & Peñuelas-Urquides, K. (in press, 2025). ***Mycobacterium susceptibility to ivermectin by inhibition of eccD3, an ESX-3 secretion system component.*** *PLOS Computational Biology*.

2022

[peer-reviewed book chapter, **First Author**] **Herrera-Rodulfo, A**., Andrade-Medina, M., & Carrillo-Tripp, M. (2022). ***Repurposing Drugs as Potential Therapeutics for the SARS-Cov-2 Viral Infection: Automatizing a Blind Molecular Docking High-throughput Pipeline.*** In biomedical Engineering. IntechOpen [Book chapter]. https://doi.org/10.5772/intechopen.105792 [free available pipeline on github]

[Review article, Co-**Author**] del Rayo Camacho-Corona, M., Camacho-Morales, A.,Góngora-Rivera, F., Escamilla-García, E., Morales-Landa, J. L., Andrade-Medina, M., **Herrera-Rodulfo, A**., García-Juárez, M., García-Espinosa, P., Stefani, T., González-Barranco, P., & Carrillo-Tripp, M. (2022***). Immunomodulatory Effects of Allium sativum L. and its Constituents against Viral Infections and Metabolic Diseases.*** In Current Topics in Medicinal Chemistry (Vol. 22, Issue 2, pp. 109–131). Bentham Science Publishers Ltd. https://doi.org/10.2174/1568026621666211122163156. 2021

2019

[Research article, **First Author**] **Herrera-Rodulfo, A**., Carrillo-Tripp, M., Laura Yeverino-Gutierrez, M., Peñuelas-Urquides, K., Adiene González-Escalante, L., Bermúdez de León, M., & Silva-Ramirez, B. (2021). ***NAT2 polymorphisms associated with the development of hepatotoxicity after first-line tuberculosis treatment in Mexican patients: From genotype to molecular structure characterizatio***n. In Clinica Chimica Acta (Vol. 519, pp. 153–162). Elsevier BV. https://doi.org/10.1016/j.cca.2021.04.017

Manuscripts in Preparation

[**Research article in preparation,** First Author] – The Role of Conformational Dynamics Conservation in the Structure-Function Paradigm: A Case Study on the RBD of SARS-CoV-2 Spike Protein Variants. In preparation.
[**Research article in preparation,** First Author] – Drug-target interaction miner, a computational framework for protein-ligand interaction analysis using modern artificial intelligence architectures and graph theory. In preparation.
[**Research article in preparation**, Co-Author] – High-Throughput Virtual Screening of Organosulfur Compounds Targeting SARS-CoV-2 Spike Protein: In Silico and In Vitro Analysis. In preparation.

Internships & Awards

Helmholtz Visiting Researcher Grant (2023) – Research stay on deep learning and graph neural networks in the Drug Bioinformatics group, Helmholtz Institute for Pharmaceutical Research Saarland (HIPS), Saarbrücken, Germany. **Molecular Modeling & Dynamics Course (2017)** – Research stay at the Biomolecular Diversity group, Center for Research and Advanced Studies (CINVESTAV), Monterrey, Mexico. **Undergraduate Research Internship** – Organic synthesis of pharmacologically active compounds, Faculty of Chemistry, Autonomous University of Nuevo León (UANL).

Selected workshops & Talks

Talks:

- Study of conserved molecular dynamics in SARS-CoV-2 spike RBD. Northeastern Biomedical Research Center (CIBIN), 2024. [**Spanish**]
- Search of molecular patterns for drug design inhibitors of SARS-CoV-2 targets. Clinical Engineering Student Group (GEIC), 2023. [**Spanish**]
- SARS-CoV-2 Spike RBD's loop conserved-dynamics. 12th Meeting on Molecular Simulations and Biophysics Week, 2023. [**English**]
- NAT2 polymorphisms and molecular dynamics in Mexican patients with tuberculosis. 2nd International Congress of Nano-bioengineering, 2020. [**English**]

Posters:

- Graph Neural Network-based prediction of drug-target interactions. International Congress of Future Biomedical Researchers, 2023. [**English**]
- High-throughput virtual screening of repurposed drugs against SARS-CoV-2. XII National Congress of Virology, 2021. [**Spanish**]
- Study of NAT2 polymorphisms in hepatotoxicity by anti-TB treatment. Symposium in honor of Dr. Jaime Kravzov Jinich, 2019. [**Spanish**]

Attendance:

- HIPS Symposium on Pharmaceutical Sciences, Saarland University, Germany, 2023. [**English**]

Teaching experience

Escuela Técnica Roberto Rocca – Open Student Projects Showcase (May 24, 2024) – Invited panelist for project evaluation. **PrepaTec** – Meeting National Scientists (April 11, 2024) – Invited to share my experience in biomedical research. **Escuela Técnica Roberto Rocca** – Science and Technology Week (June 8-9, 2022) – Conducted a workshop to reinforce students' understanding of microorganism size scale using audiovisual material, graphic novels, and paper models. **CINVESTAV** – Master's in Biology Education for Citizenship Formation (2022-2024) – Participated in classes and workshops focused on education through seminars, mentoring, and hands-on activities.

Overview of main Research projects

Exploring how conservation in the molecular dynamics can reveal functional regions critical for therapeutic targeting (2024). We investigated whether the SARS-CoV-2 receptor binding domain maintains both its structural and dynamic properties across variants, and examined if this conservation relates to function. Through rigorous and systematic analysis of evolutionary variants, we aimed to identify critical functional regions that could serve as therapeutic targets.

Developing an in-house tool for the analysis of target-ligand binding patterns (2023). We developed a bioinformatic tool, crafted in pytorch that integrates custom modules to cast target-ligand binding interactions from 3D coordinates complex and generate molecular graphs of most-frequent binding patterns using graph mining algorithms. Including modules focused on binding site and ligand molecular structure (SAR -like analysis).

Automatizing a Blind Molecular Docking High-throughput Pipeline (2021). Development of an in-house tool for high-throughput molecular docking. The tool is crafted in bash and integrates a custom pipeline to run molecular docking analysis of protein-ligand complexes until they converge to minimal binding score prediction.

Understanding the effect of non-synonymous mutations on protein function (2019). We studied the effect of single-nucleotide polymorphisms in NAT2 protein structure through in-vitro experiments and a robust computational modelling pipeline and proposed a feasible explanation for slow acetylation rates on NAT2 due to non-synonymous mutations.

Contact information of academic references

Dr. Mauricio Carrillo Tripp
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https://tripplab.com/

Dra. Beatriz Silva Ramirez
[Master's advisor: silbear2002@yahoo.es]