Aldo Herrera Rodulfo

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EDUCATION

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CENTER FOR RESEARCH AND ADVANCED STUDIES (CINVESTAV MTY) Apodaca, Mexico
PhD, In Science, Engineering and Biomedical Physics **29- Ago-2025**
Thesis: *Conformational dynamics of the RBD in SARS-CoV-2 variants: Functional conservation in a changing evolutionary landscape*

AUTONOMOUS UNIVERSITY OF NUEVO LEON (FCQ, UANL) San Nicolás, Mexico
Master's in Science with a focus on Pharmacy**, GPA: 3.95** **12-Ago-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 LEON (FCQ, UANL) San Nicolás, Mexico
Bachelor's in Science: **Pharmaceutical Biologist Chemist, GPA: 3.40** **Jun-2018**

RESEARCH VISITS

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Research stay at Helmholtz Institute for Pharmaceutical Research Saarland (HIPS) Saarbrücken, Germany
Graph-driven deep learning for mapping drug–target interaction networks **May-Ago 2023**

Research stay at Center for Research and Advanced studies (CINVESTAV MTY) Apodaca, Mexico
Molecular modelling & dynamics, data generation and analysis from HPC simulations **Oct 2019- Ago 2020**

Research stay at Natural Products Chemistry Laboratory, CELAES, FCQ, UANL San Nicolás, Mexico
Organic synthesis of compounds with potential pharmacological activity. **Jun 2017 - Dic 2017**

SKILLS

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Computational Biophysics: Molecular dynamics (GROMACS, enhanced sampling methods: AWH, umbrella sampling, free energy perturbations: MM/PBSA, FEP, Coarse-grained, OpenMM, CHARMM, MDAnalysis, MDTraj, cluster analysis), chemoinformatics and drug design (GNN, MGL tools, AutoDock Vina, CB-Dock, HADDOCK, PLIP, OpenBabel, RDKit, ODDT, QSAR).

Structural Analysis & Molecular Modeling: PyMOL, VMD (Tk Console), ChimeraX (CLI), Avogadro, ChemDraw; molecular modeling tools include Rosetta, Swiss-Model, UCSF Chimera, AlphaFold3, RoseTTAFold.

Protein Design & Engineering: RFdiffusion, RoseTTAFold, Boltz-2, ProteinMPNN; sequence analysis: BLAST, MUSCLE.

Databases: BindingDB, BioLiP2, PLAS20K, MISATO.

Coding & HPC: Python, R, Bash, Nextflow; data analysis and visualization: Pandas, Matplotlib, Seaborn, NumPy, SciPy, Scikit-learn; machine learning: PyTorch, TensorFlow; HPC: Slurm, TMUX, Linux/Unix systems.

Wet Lab Techniques: DNA/RNA extraction and purification, PCR, bacterial culture, protein expression and purification, spectrophotometry (UV-Vis, NanoDrop).

Soft Skills: Curious, creative, team player, willing to learn, supportive, proactive, adaptable, resourceful, resilient, independent, organized, empathetic, collaborative, results-driven.

Languages: Spanish (native), English (C1, conversational).

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 (here) & Protein-Ligand molecular dynamics simulations (here).

PUBLICATIONS

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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.

SELECTED WORKSHOPS & TALKS

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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**]

OVERVIEW OF FIRST-AUTHOR RESEARCH PROJECTS

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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.

OUTREACH EXPERIENCE

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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 with students.

Escuela Técnica Roberto Rocca – Science and Technology Week (June 8–9, 2022) – Conducted a workshop to help high-school students understand microorganism size scales using audiovisuals, graphic novels, and paper models.

CINVESTAV – Master's in Biology Education for Citizenship Formation (2022–2024) – Participated in seminars, mentoring, and hands-on activities focused on science education.

Participation on outreach projects

> **"Who Stole the Virus?" (2022 & 2023) –** Contributed to a didactic course combining in-vitro and in-silico approaches to solve a scientific mystery. Provided consulting, conferences, and workshops on bioinformatic analysis of genomic sequences.
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> **"How Small a Virus Is?" (June 2022) –** Helped high-school students explore the scale of microscopic entities through audiovisuals, storyboards, and paper virus models during Science, Art, and Technology Week.
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> **"What Motivated Me to Do Science?" –** Shared my experience as a science student with future biology teachers, guiding discussions and helping analyze student-generated data (drawings) on motivations for pursuing science.

Aldo Herrera Rodulfo, PhD
More about me: aldhr.github.io/

If you only do what you can do, you'll never be better than what you are
- Master Shifu, Kung fu panda 3 (2016)