Aldo Herrera-Rodulfo, PhD.

Computational Biologist | Interested at the intersection of protein dynamics, evolutionary patterns, and molecular mechanisms driving biological function.

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Media: *Linkedin* – *Google scholar* – *ResearchGate* – *X*

Education

→ PhD, Engineering and Biomedical physics **August, 2025**
Center For Research and Advanced Studies (CINVESTAV)
Thesis: **Conformational dynamics of the RBD in SARS-CoV-2 variants: Functional conservation in a changing evolutionary landscape**

→ MSc, Pharmaceutical Sciences **August, 2020**
Autonomous University of Nuevo Leon (UANL)
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.**

→ BSc, Pharmaceutical Biologist Chemist **July, 2018**
Autonomous University of Nuevo Leon (UANL)

Publications (6)

→ 2025

[Research article, 2nd Author] Martha Susana García-Delgado, **Herrera-Rodulfo, A.,** Karen Y Reyes-Melo, Ashly Mohan, Fernando Góngora-Rivera, Jesús Andrés Pedroza-Flores, Alma D. Paz-González, Gildardo Rivera, María del Rayo Camacho-Corona*, Mauricio Carrillo-Tripp*. ***A Garlic-Derived Lead Compound Targeting SARS-CoV-2 Entry via RBD-ACE2 Disruption.*** (In press, 2025). Molecules MDPI.

[Research article, 1st Author] **Herrera-Rodulfo, A.**, Andrade-Medina, M., García-Delgado, M. S., & Carrillo-Tripp, M. (2025). **Extensive In-silico Target-Ligand Conformational Space Sampling of Garlic-Derived Sulfur Compounds Targeting COVID-19 Infection.** Journal of Computational Biophysics and Chemistry, 25(07), 1033–1051. https://doi.org/10.1142/s2737416525500267

[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. (2025). **Mycobacterium susceptibility to ivermectin by inhibition of eccD3, an ESX-3 secretion system component.** PLOS Computational Biology, 21(4), e1012936. https://doi.org/10.1371/journal.pcbi.1012936

→ 2023

[Peer-Reviewed Book Chapter, 1st Author] **Herrera-Rodulfo, A.,** Andrade-Medina, M., & Carrillo-Tripp, M. (2023). **Repurposing Drugs as Potential Therapeutics for the SARS-Cov-2 Viral Infection: Automatizing a Blind Molecular Docking High-throughput Pipeline.** In Biomedical Engineering. IntechOpen. https://doi.org/10.5772/intechopen.105792

→ 2022

[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

[Research Article, 1st 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 characterization.** In Clinica Chimica Acta (Vol. 519, pp. 153–162). Elsevier BV. https://doi.org/10.1016/j.cca.2021.04.017

Research Experience

→ Molecular modelling

- **Modeled structural impacts of SNPs in enzymes** (incl. NAT2), **linking residue substitutions within structural and dynamical alteration**, describing their effect on protein function to **explain clinical outcomes.**
- Characterized non-synonymous changes, insertions, and deletions in viral variant proteins to **study the effect of these changes in infectious variants on protein dynamics and evolutionary behavior.**
- **Designed a pipeline** to identify conserved residues at **protein-protein interfaces**, pinpointing key sites relevant to function for **therapeutic targeting.**
- Supported collaborative projects by **generating and preparing large, structured datasets for high-throughput molecular docking campaigns.**
- **Applied molecular modeling to diverse biological systems contributing structural insights to interdisciplinary teams.**

→ Molecular dynamics

- **Designed and executed advanced MD simulation pipelines** (GROMACS; AWH, umbrella sampling, free energy calculations (PMF); coarse-grained models; protein-ligand simulations).
- **Developed a dedicated pipeline to assess conservation of dynamics across protein variants**, incorporating RMSD/RMSF similarity metrics, PCA/essential dynamics, clustering, free-energy landscapes, and interaction-network comparison.
- Performed steered molecular dynamics (SMD) simulations to **induce and study large-scale conformational changes,** such as protein domain opening. **Reconstructed the potential of mean force (PMF) along the pulling coordinate to quantitatively characterize the energetics** of the gating mechanism.
- **Developed and executed semi-automated pipelines for comprehensive protein-ligand MD studies**, from initial ligand parametrization and system setup to production simulations and post-processing analysis.
- **Integrated structural, evolutionary, and dynamic data to pinpoint conserved functional regions** to identify dynamic hotspots relevant for therapeutic targeting.
- Managed **end-to-end simulation workflows on HPC clusters using Slurm and TMUX for large-scale simulation campaigns.**

→ Graph representation of molecular fingerprints of Protein-Ligand Binding patterns

- **Curated large biochemical datasets** (BindingDB, BioLiP2, PLAS20K, MISATO) to **assemble reliable training/validation sets.**
- **Engineered atomic-level and ligand-substructure features into molecular graphs to capture protein-ligand interaction patterns,** by implementing PyTorch modules for molecular graph construction and feature embedding.
- **Built a complete computational pipeline to convert 3D protein-ligand complexes into molecular interaction graphs** suitable for Graph Neural Networks (GNNs), **incorporating SAR-like analysis modules for binding site and ligand molecular structure characterization.**

Research Visits

→ 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

Technical Skills

Computational Biophysics: Molecular dynamics (GROMACS, steered-MD, enhanced sampling methods: AWH, umbrella sampling, PMF, free energy landscape, Coarse-grained, MDTraj, cluster analysis), chemoinformatics and drug design (GNN, MGL tools, AutoDock Vina, CB-Dock, PLIP, OpenBabel, RDKit). **Structural Analysis & Molecular Modeling:** PyMOL, VMD (Tk Console), ChimeraX (CLI), Avogadro, Rosetta, Swiss-Model, UCSF Chimera, AlphaFold3, RoseTTAFold. **Sequence analysis:** BLAST, MUSCLE, Clustal Omega. **Databases:** BindingDB, BioLiP2, PLAS20K, MISATO. **Coding & HPC:** Python, R, Bash, Slurm, TMUX, Linux/Unix systems. **Data analysis and visualization:** Pandas, Matplotlib, Seaborn, NumPy, SciPy, Scikit-learn, Pytorch. **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. **See my coding portfolio** here.

Selected Workshops, Talks & Outreach

→ 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

Biogenix – Instructor (November 2025) – Taught Sequence alignment and ensemble algorithms in a professional course setting.

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.

More about me: aldhr.github.io/