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Aldo Herrera Rodulfo

April 25, 1996.

Monterrey, México

EDUCATION

>PhD in Engineering and Biomedical Physics.

Biomolecular Diversity Lab at the Center for Research and Advanced Studies (CINVESTAV). 2020-2024

- *Project*: Computational study of the SARS-CoV-2 spike protein in search of ligand binding sites for the design of viral entry inhibitors.
- *Secondary project*: Repurposing Drugs as Potential Therapeutics for the SARS-Cov-2 Viral Infection: Automatizing a Blind Molecular Docking High-throughput Pipeline

>Master in science focused on pharmacy.

Immunogenetics lab at Northeast Biomedical Research Center (CIBIN, IMSS). Faculty of Chemistry at Autonomous University of Nuevo León (UANL).

2018-2020

- *Project*: Analysis of N-acetyltransferase 2 (NAT2) gene polymorphisms as markers of liver damage by first-line pulmonary tuberculosis treatment in a northeastern Mexican population and molecular dynamics studies.

>Bachelor in chemistry applied to biological and pharmaceutical sciences. Faculty of Chemistry at Autonomous University of Nuevo León (UANL).

2013-2018

RESEARCH VISIT

>HIDA - helmholtz visiting researcher grant holder.

Drug Bioinformatics at Helmholtz Institute for Pharmaceutical Research Saarland (WIBI, HIPS). Saarbrücken, Germany - 2023

- *Project*: Graph Neural Networks to identify potential drugs for SARS-CoV-2 using explainability models to understand drug-protein interactions.

CONTACT DETAILS

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PEER-REVIEWED PUBLICATIONS

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

- **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

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. F.**, 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

CONFERENCE PRESENTATIONS

Talks

- **Herrera-Rodulfo A.**, & Carrillo-Tripp, M. (2023) "Search of molecular patterns for the rational design of drugs as inhibitors of SARS-CoV-2 targets". Clinical Engineering Student Group (GEIC). Science and Engineering Division (DCI). [certificate]

- **Herrera-Rodulfo A.**, Carrillo-Tripp M. (2023) "SARS-CoV-2 Spike RBD's loop conserved-dynamics show potential for developing new therapeutics" (2023) presented at 12th Meeting on Molecular Simulations and virtual biophysics student forum of Biophysics Week. [certificate]

- Vásquez-Cerqueda I.D., & **Herrera-Rodulfo A.** (2022) "How do we represent small biological entities? The stereotype of the human cell. "XI Latam congress of the teaching of biology and environmental education. Approaches to the problems and needs of the region" 27-28 Oct. Virtual modality. Narrative of teaching experience. [certificate]

- **Herrera-Rodulfo A.**, & Carrillo-Tripp, M. (2020) "Single-nucleotide polymorphisms analysis and molecular dynamics of NAT2 variants from northeast mestizo-mexican patients with pulmonary tuberculosis, and the ones who develop hepatotoxicity after the first-line anti-tubercular regimen." in the 2nd international congress of Nano-bioengineering in the virtual forum of biotechnology and nanotechnology research. 24-30 Oct. Monterrey city. [certificate]

Poster

- **Herrera-Rodulfo A.**, & Carrillo-Tripp, M. (2021) "High-throughput virtual screening of repurposed drugs against SARS-CoV-2 cell recognition and entry, polyprotein processing, and RNA replication phases" in the XII National congress of virology of mexican society of virology. 29 Sep – 2 Oct, Monterrey city. [certificate].
- **Herrera-Rodulfo A.**, Yeverino-Gutierrez M., Silva-Ramírez B. (2019) "The study of NAT2 polymorphisms in their role in hepatotoxicity by anti-TB treatment" in the symposium in honor of Dr. Jaime Kravzov Jinich " innovation in pharmaceutical sciences". 11-13 Nov. México City. [certificate]

Attendance

- Institute for Pharmaceutical Research Saarland (HIPS) Symposium (2023) on pharmaceutical sciences devoted to infection research. **Saarland University Campus in Saarbrücken, Germany**. [certificate]

ABOUT ME

In my spare time, I enjoy discovering movies and series. I usually try to avoid reading synopses. I'm also a co-founder of a two-member book club with my fiancée and unfortunately I think more often about playing sports than I actually do. My favorites? Soccer and tennis.

SKILL SET

Here, I'll list a *few* examples of tools that I'm familiar with:

>**Languages**

- Spanish [Native], English [Proficient]

>**Programming language**

- Python, R, Bash (LINUX/UNIX)

>Tools for **molecular simulation**

- GROMACS
    - Cluster analysis
    - RMSF and PCA analysis

>Tools for **molecular docking**

- Autodock VINA, MGL tools
    - Curation of dataset
    - Automatization of the process

>Tools for **molecular modeling**

- Chimera UCSF, ROSETTA, Alpha fold
    - template-based modeling
    - mutation of residues
    - loop modelling

>Tools for **chemoinformatics**

- Rdkit, Open Babel
    - Analysis of chemical descriptors (MW, logP, pKa, ...)

>Tools for **bioinformatics**

- MUSCLE, BLAST
    - Alignment of sequences
    - Identity analysis

>Tools for **deep learning**

- Pytorch, Scikit-learn, Neural Network Architectures

Other activities

I also enjoy participating in activities related to teaching science and divulgation. Here I'll list a few projects that I was lucky to be part of.

>Who stole the virus? | I helped to solve a mystery at the BMD lab. I have participated in two editions (2022 and 2023) of "Who stole the virus?". A didactic course that employs in-vitro and in-silico tools to solve a well-planned mystery by master's students of the master program in biology education for citizen formation at the Center of Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV-IPN). My contribution includes day-to-day consulting and conferences and workshops on bioinformatic analysis of genomic sequences.

>How small a virus is? | How do students perceive the size of small entities?. Sometimes the size of the biological world is not as intuitive as we think. I was part of a team that help out high-school students to deeper understand how small entities are more fun than they thought, we used audiovisuals, graphic storyboards, paper virus models at the **week of science, art and technology** at Roberto Rocca technical school (8 and 9 of June 2022) in a workshop named: "A trial to a virus: the small and the very small"

>What motivated me to do science? | I shared my experience with the future teachers of biology students.

I was invited as a member of the Biomolecular Diversity Lab to share my experience as a science student. I share my motivations to do science, and what I enjoy about it. Then, I also helped the project-leaders to analyze the results of this course (throughout biology trainee teachers drawings!). This was part of a course of nature of sciences at the benemerit and centenary school for future teachers of Jalisco (ByCENJ).