last update: Dic 20 2023

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*: Identification of regions with conserved dynamics involved in key conformational changes for SARS-CoV-2 protein S activation as therapeutic target for drug design.

>*Master in science focused on pharmacy.*

Immunogenetics lab at Northeast Biomedical Research Center (CIBIN, IMSS) and the Faculty of Chemistry at Autonomous University of Nuevo León (FCQ, 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

Email: aldo.hrodulfo@gmail.com

RxGATE | Google Scholar | ORCID | Github | linkedin

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]

Herrera-Rodulfo A., Kalinina O., Carrillo-Trip M. (2023) "Graph Neural Network-based prediction of essential interactions on drug-target complexes" International congress of future biomedical researchers. 15-17 Nov. San Nicolás de los Garza. [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 like to watch movies and series, but I don't have any particular favorite movie genre; I just try to surprise myself. That's why I don't usually read synopses. I also co-founded a book club with my fiancée, but sometimes it's hard to keep up, but I try my best not to get expelled.

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
    - Molecular dynamics simulation of biological systems
    - Trajectory processing and analysis

>Tools for **molecular docking**

- Autodock VINA, MGL tools
    - Quality assessment
    - Automatization of the molecular docking

>Tools for **molecular modeling**

- Chimera UCSF, ROSETTA, Alpha fold
    - homology modeling
    - In-silico mutations

>Tools for **chemoinformatics**

- Rdkit, Open Babel
    - Analysis of chemical structure and molecular descriptors (MW, logP, PSA, ...)

>Tools for **bioinformatics**

- MUSCLE, BLAST
    - Alignment of sequences and identity analysis

>Tools in **python**

- Deep learning architectures, Data Wrangling, Data Visualization
    - Pytorch, Scikit-learn, Scipy, Numpy, Pandas
    - Matplotlib, Seaborn, Plotly

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).