ALDO HERRERA RODULFO

Computational Biologist, PhD.

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https://aldhr.github.io/

EXPERIENCE

Computational Biologist | 2018-2024

- **Molecular Modelling & Simulations**
  - Strong problem-solving skills for designing experiments and simulations to address key research questions.
  - Extensive experience in biomolecular simulations for protein conformational sampling.
  - Experience within multimonomeric protein assembies and protein-ligand simulations and analysis.
  - Experience in advance protocols for enhanced sampling methods for free-energy estimations and conformational transitions.
  - Skilled in high-throughput virtual screening pipelines and molecular docking.
  - Proficient with cheminformatics software for molecular modeling and handling large-scale chemical databases.
- **Programming Workflows**
  - Experienced in managing and curating large datasets for computational biology and cheminformatics applications.
  - Strong Python and R programming skills with extensive bash scripting experience for automating molecular docking and dynamic simulations.
  - Developed modular, reusable workflows for high-throughput simulations and bioinformatics tasks.
  - Proficient with cloud computing environments and Linux/UNIX tools.
- **Communication Skills**
  - Ability to interpret complex biological data and develop computational analysis to address key research questions.
  - Excellent oral and written communication skills, with a track record of publishing in peer-reviewed journals and presenting at international conferences.
  - Proven ability to explain complex topics to interdisciplinary teams and a collaborative mindset, working effectively with experts from various fields.

EDUCATION

2020- 2024
PhD in Biomedical Physics and Engineering.
Center for Research and Advanced Studies (CINVESTAV)

2018 - 2020
MSc. in pharmacy
Autonomous University of Nuevo Leon (UANL)

2013 - 2018
BSc. in chemist pharmaceutical biologist
Autonomous University of Nuevo Leon (UANL)

RESEARCH VISITING

2023
PhD research visiting on graph neural networks for mining protein-ligand binding patterns
Helmholtz institute for pharmaceutical research (HIPS)

2018
Practical and Theoretical Course on Molecular Modeling and Dynamics
Center for Research and Advanced Studies (CINVESTAV)

2017
Undergrad Research Internship on organic synthesis of potential anti-cancer molecules.
Autonomous University of Nuevo Leon (UANL)

PEER-REVIEWED PUBLICATIONS

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.** IntechOpen. doi: 10.5772/intechopen.105792

Del Rayo Camacho-Corona M, Camacho-Morales A, Góngora-Rivera F, Escamilla-García E, Morales-Landa JL, Andrade-Medina M, **Herrera-Rodulfo AF**, García-Juárez M, García-Espinosa P, Stefani T, González-Barranco P, Carrillo-Tripp M. **Immunomodulatory Effects of Allium sativum L. and its Constituents against Viral Infections and Metabolic Diseases**. Curr Top Med Chem. 2022;22(2):109-131. doi: 10.2174/1568026621666211122163156. PMID: 34809549.

Herrera-Rodulfo A, Carrillo-Tripp M, Laura Yeverino-Gutierrez M, Peñuelas-Urquides K, Adiene González-Escalante L, Bermúdez de León M, Silva-Ramirez B**. NAT2 polymorphisms associated with the development of hepatotoxicity after first-line tuberculosis treatment in Mexican patients: From genotype to molecular structure characterization**. Clin Chim Acta. 2021 Aug;519:153-162. doi: 10.1016/j.cca.2021.04.017. Epub 2021 Apr 29. PMID: 33932406.

TALKS & POSTERS

- Study of conserved molecular dynamics in SARS-CoV-2 spike RBD. Northeastern Biomedical Research Center (CIBIN), 2024. [**Talk**]
- Search of molecular patterns for drug design inhibitors of SARS-CoV-2 targets. Clinical Engineering Student Group (GEIC), 2023. [**Talk**]
- SARS-CoV-2 Spike RBD's loop conserved-dynamics. 12th Meeting on Molecular Simulations and Biophysics Week, 2023. [**Talk**]
- NAT2 polymorphisms and molecular dynamics in Mexican patients with tuberculosis. 2nd International Congress of Nano-bioengineering, 2020. [**Talk**]
- Graph Neural Network-based prediction of drug-target interactions. International Congress of Future Biomedical Researchers, 2023.[**Poster**]
- High-throughput virtual screening of repurposed drugs against SARS-CoV-2. XII National Congress of Virology, 2021. [**Poster**]
- Study of NAT2 polymorphisms in hepatotoxicity by anti-TB treatment. Symposium in honor of Dr. Jaime Kravzov Jinich, 2019. [**Poster**]
- HIPS Symposium on Pharmaceutical Sciences, Saarland University, Germany, 2023. [Attendence]

BIOINFORMATIC PIPILINES

Bash-Scripting Pipeline: Automates multiple-cycle molecular docking analysis, processes files into AutoDock VINA inputs, formats output into CSV for further analysis.

Graph-Embedding for protein-ligand profiling: Extracts protein-ligand information from PDB IDs into graph format for Graph Neural Network input.

Python Notebooks: Analyzes distribution of molecular docking sets, visualizes protein frequent electrostatic interactions.

RESEARCH UNDER PEER-REVIEWING PROCESS.

Co-author
Mycobacterium susceptibility to ivermectin by inhibition of eccD3, ESX-3 secretion system component.

First-author
Extensive In Silico T arget – Ligand Conformational Space Sampling of Garlic-Derived Sulfur Compounds targeting COVID-19 infection

First-author
Identification of potential sites in the SARS-CoV-2's receptor binding domain for preventing viral infection.

LANGUAGES

English (Professional proficient)
Spanish (Native)