Aldo Fernando Herrera Rodulfo

mail aldo.hrodulfo@gmail.com
web https://aldhr.github.io
github https://github.com/aldhr

Profile

Highly motivated and skilled scientist with a Ph.D. in Biomedical Physics and Engineering, specializing in computational biology. Expertise in molecular dynamics simulations with experience in enhanced sampling methods and free energy estimations and virtual screening, with a focus on drug discovery. Proven track record of scientific achievements, including publications in peer-reviewed journals. Strong analytical, hypothesis-generator, problem-solving, and teaching and collaborative skills.

Skill Set

Molecular Dynamics Simulations:

- Extensive experience with advanced GROMACS protocols, including simulations of protein assemblies with multiple monomer units, protein-ligand interactions, free energy estimations, umbrella sampling, and adaptive biasing.

Virtual Screening:

- Expertise in molecular docking analysis, implementing a high-throughput bash pipelines to assess a customizable number of ligands against selected protein sites across multiple cycles [code].
- Skilled in the systematic analysis of protein-ligand interactions using third-party tools (such as, protein-ligand interaction profiler and Rdkit) in a python-written analysis notebooks [code]
- Contributed to the implementation of a cavity-guided blind docking high-throughput bash pipeline, published as a peer-reviewed chapter [DOI].

Bioinformatics:

- Developed scripts for automating tasks such as (1) batch downloading PDB structures from RCSB (2) parsing PDB information into tabular formats using pandas, (3) extracting SMILE and FASTA sequences from PDB, and (4) converting mol2 files to PDB while preserving secondary structure and more... [codes]

Structural Bioinformatics:

- Designed and implemented a tool to parse protein-ligand PDB structures, extract protein interacting residues, analyze intermolecular interactions, and create heterogeneous graphs for mining frequent binding patterns.

Software Skills:

- **Molecular modelling & dynamics:** GROMACS, MDAnalysis, VMD, Chimera UCSF, AutoDock VINA, CB-Dock, MGLTools, PyMol, Rosetta software, AlphaFold, RFdiffusion, LIGPLOT, swiss-model, Avogadro, BIOVIA.

- **Programming & Tools:** Python, R, Bash-Scripting, VIM, tmux (LINUX/UNIX); GenBank, Biopython, EMBL-tools, PROSITE, T-coffee, Rdkit, Openbabel, Numpy, Pandas, Matplotlib, Seaborn, Plotly, Scikit-learn, Pytorch.

Education

- **PhD in Biomedical Physics and Engineering** | 2020 - Present
  Biomolecular Diversity Lab, Center for Research and Advanced Studies (CINVESTAV).

- **Master in Science focused on pharmacy** | 2018 - 2020
  Immunogenetics Lab, Northeast Biomedical Research Center (CIBIN, IMSS) & Faculty of Chemistry, Autonomous University of Nuevo León (FCQ, UANL).

- **Bachelor in Chemistry Applied to Biological and Pharmaceutical Sciences** | 2013 - 2018
  Faculty of Chemistry, Autonomous University of Nuevo León (UANL).

Research Publications

- **First-Author Publications:**
  - 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. Biomedical Engineering. IntechOpen. DOI

    - Herrera-Rodulfo, A., et al. (2021). NAT2 polymorphisms associated with hepatotoxicity after first-line tuberculosis treatment in Mexican patients. Clinica Chimica Acta, 519, 153–162. Elsevier BV. DOI

- **Co-Author Publications:**
    - del Rayo Camacho-Corona, M., et al. (2022). Immunomodulatory Effects of Allium sativum L. against Viral Infections and Metabolic Diseases. Current Topics in Medicinal Chemistry, 22(2), 109–131. Bentham Science Publishers. DOI

Internships & Awards

- **Helmholtz Visiting Researcher Grant** | 2023
  Research stay on deep learning graph-neural networks, Drug Bioinformatics group at Helmholtz Institute for Pharmaceutical Research Saarland (HIPS), Saarbrücken, Germany.
- **Practical and Theoretical Course on Molecular Modeling and Dynamics** | 2019
  Biomolecular Diversity Group, Center for Research and Advanced Studies (CINVESTAV), Monterrey, Mexico.
- **Undergrad Research Internship** | 2017
  Organic Synthesis Lab, Faculty of Chemistry, Autonomous University of Nuevo León (FCQ, UANL).

Useful Scripts in Bioinformatics Analysis

- **Bash-Scripting Pipeline:** Automates multiple-cycle molecular docking analysis, processes files into AutoDock VINA inputs, formats output into CSV for further analysis. GitFront
- **Python Notebooks:** Analyzes distribution of molecular docking sets, visualizes protein frequent electrostatic interactions. GitFront
- **Graph-Embedding Codes:** Extracts protein-ligand information from PDB IDs into graph format for Graph Neural Network input. GitFront

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Workshops, Conferences, and Posters

- **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]