Aldo Herrera Rodulfo

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Computational biologist specializing in protein structure, molecular dynamics, and drug discovery. Expertise in high-throughput bioinformatics pipelines, AI-driven structural predictions, and ligand-binding protein analysis. Proven track record in developing computational frameworks for therapeutic research, with a strong interest in collaborative, cutting-edge innovations in protein design. Passionate about translational research in an entrepreneurial setting to advance biomedicine.

RELEVANT TECHNICAL SKILLS

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

Programming packages in bioinformatics & chemoinformatics. GenBank, Biopython, EMBL-tools, PROSITE, T-coffe, Rdkit, Openbabel, Numpy, Pandas, Matplotlib, Seaborn, Plotly, Scikit-learn, Pytorch

Programming languages. Python, R, Bash-Scripting, VIM, tmux (LINUX/UNIX)

Other skills: Can be found at my online resume: https://aldhr.github.io

RESEARCH EXPERIENCE

Exploring how conservation in the molecular dynamics can reveal functional regions critical for therapeutic targeting 2024

- We investigated whether the SARS-CoV-2 receptor binding domain maintains both its structural and dynamic properties across variants, and examined if this conservation relates to function. Through rigorous and systematic analysis of evolutionary variants, we aimed to identify critical functional regions that could serve as therapeutic targets.

Developing an in-house tool for the analysis of target-ligand binding patterns. 2023

- > This is crafted in python and integrates custom modules to cast target-ligand binding interactions from 3D coordinates complex and generate molecular graphs of most-frequent binding patterns using graph mining algorithms. Including modules focused on binding site and ligand molecular structure (SAR -like analysis).

Automatizing a Blind Molecular Docking High-throughput Pipeline 2021

- Development of an in-house tool for high-throughput molecular docking.
  > This is crafted in bash and integrates a custom pipeline to run molecular docking analysis of protein-ligand complexes until they converge to minimal binding score prediction.

RESEARCH EXPERIENCE

Understanding the effect of non-synonymous mutations on protein function 2019

- We studied the effect of single-nucleotide polymorphisms in NAT2 protein structure through a robust computational modelling pipeline and proposed a feasible explanation for slow acetylation rates on NAT2 due to non-synonymous mutations.

EDUCATION

PhD in Engineering and biomedical physics - CINVESTAV, México 2025
MSc in Pharmacy sciences - UANL, México 2020
BSc in Biopharmaceutical chemistry - UANL, México 2018

INTERNSHIPS & AWARDS

Honored to be awarded the HIDA's Helmholtz Visiting Researcher Grant. 2023
Practical and theoretical course on molecular modeling and dynamics. 2019
Undergrad internship at drug and natural product synthesis lab 2017

PUBLICATIONS

[peer-reviewed book chapter] **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 [free available pipeline on github]

[Review article] 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] **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 characterizatio***n. In Clinica Chimica Acta (Vol. 519, pp. 153–162). Elsevier BV. https://doi.org/10.1016/j.cca.2021.04.017