Alma C. Castañeda-Leautaud

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Research Interests

My main interest is in drug design and structural biology at the atomic level. I currently focus on applying deep learning, particularly Graph Neural Networks (GNNs), to process large virtual screening libraries and explore chemical space through clustering and dimensionality reduction. I also employ molecular simulations and free energy calculations to study protein–ligand interactions and mechanistic phenomena. A central challenge of my work is to perform large-scale chemical space exploration and long-timescale simulations through optimized and automated GPU-accelerated workflows.

Education

Ph.D. Candidate in Chemistry

GPA: 3.8, UCSD, San Diego, CA, USA, (2022–Present)

Thesis: *GNN-Driven Drug Design and Translocation Mechanism of SARS-CoV-2 NSP13*
PI: Prof. Rommie Amaro

M.Sc. Nanosciences

CICESE, Ensenada, B.C., México (2017–2020)

Thesis: *Proposal of a new antipsychotic free of cardio metabolic side sffects by molecular dynamics*
PI: Prof. Sergio Águila Puentes

B.S. Nanotechnology

UNAM, Ensenada, B.C., México (2012–2017)

Thesis: *Disassembly and reassembly of an icosahedral virus*
PI: Prof. Rubén Darío Cadena Nava

Languages

- Spanish (Native)
- English (TOEFL iBT 121, 2020)
- German (A2, 2015)

Honors & Awards

- Fulbright-García Robles Scholarship, USA (2022–2025)
- CONACYT Scholarship, France (2020)
- CONACYT Scholarship, México (2017–2019)

Work & Research Experience

Research Intern

Midwest Antiviral Drug Discovery (AViDD) Center, USA (2023–2025)

Research:
- Virtual screening–based drug discovery and binding site identification for Nsp13 helicase.

Biotesting Lab Coordinator

Quality Control Department, Biotix, México (2021–2022)

Research:
- Automated PDF certificate generation synchronized with databases.
- Performed sterilization testing using micro and molecular biology techniques.

Publications

1. Castañeda Leautaud, A. C., & Amaro, R. (2025). *Optimal message passing for molecular prediction is simple, attentive, and spatial.* Digital Discovery (under review).

2. Castañeda Leautaud, A. C., Srivastava, A., Eun Jung, K., Chung, D., Bannister, T. D., & Amaro, R. E. (2025). *Discovery of tetrahydroisoquinoline-based SARS-CoV-2 helicase inhibitors with iterative, deep learning enhanced virtual screening.* J. of Chem. Inf. and Model. (under review).

3. Castañeda-Leautaud, A. C., Vidal-Limón, A., & Águila, S. A. (2022). *Molecular dynamics and free energy calculations of clozapine bound to D2 and H1 receptors.* J. of Biom. Struct. and Dynam., 41(19), 9313–9325. doi.org/10.1080/07391102.2022.2148748

4. Petranovsky, V., & Castañeda, A. (2013). *Factores que influencian la presión y temperatura en el sistema solar.* La Gaceta UNAM, 16, 5–6.

Conferences

- ACS Spring National Meeting, San Diego (2025), poster
- Gulf Coast Undergraduate Research Symposium, Rice Univ. (2021), speaker

- PRONABES Fellowship, México (2012–2016)
- III Coloquio de Simulaciones Computacionales (2020), speaker
- Symposium of Nanoscience and Nanomaterials (2020, 2019), speaker/poster

Technical Skills

Programming:

Python, Bash, C-shell

Python Libraries:

- **Data & Visualization:** NumPy, CuPy, pandas, matplotlib, seaborn, PIL, scikit-learn
- **Deep Learning:** PyTorch, PyTorch Geometric, Optuna
- **Cheminformatics:** RDKit, MolVS, Mendeleev
- **Utilities:** os, re, logging, tqdm, etc.

Molecular Modeling:

AMBER, NAMD, VMD, CHARMM-GUI, AutoDock, Schrödinger Suite, MDAnalysis, ProDy, Open Babel

Other:

MATLAB, SolidWorks, Mathematica, Quantum ESPRESSO

Courses & Training

Programming & Data Science

- Python Data Structures (UMich, 2021)
- Accessing Web/Network Data (UMich, 2021)
- Advanced Python (DataCamp, 2020)
- Python 101 for Data Science (IBM, 2020)
- Applied Data Science with Python (IBM, 2020)
- Data Mining (III Coloquio en Simulaciones Computacionales, 2020)

Computational & Physical Sciences

- Molecular Dynamics (UNAM, 2018)
- Ferromagnetic Fluids (Clubes de Ciencia, 2015)
- Topological Phases (Clubes de Ciencia, 2014)