Alma C. Castañeda-Leautaud

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Research Interests

- AI-Driven Drug-Design
- Exploration of the Synthesizable chemical space
- Enhanced Molecular simulations
- Free energy calculations
- GPU-accelerated workflows in Chemistry

Education

Ph.D. Candidate in Chemistry

GPA: 3.8, UC 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 Score: 121, 2020), and German (A2, 2015).

Honors & Awards

- Fulbright-García Robles Scholarship, USA (2022–2025)
- CONACYT Scholarship, France (2020)
- CONACYT Scholarship, México (2017–2019)
- PRONABES Fellowship, México (2012–2016)

Work & Research Experience

Research Intern

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

Biotesting Lab Coordinator

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

Conferences

- ACS Spring National Meeting, San Diego (2025), poster
- Gulf Coast Undergraduate Research Symposium, Rice Univ. (2021), speaker
- III Coloquio de Simulaciones Computacionales (2020), speaker
- Symposium of Nanoscience and Nanomaterials (2020, 2019), speaker/poster

Publications

1. Castañeda Leautaud, A. C., & Amaro, R. (2025). *Optimal message passing for molecular prediction is simple, attentive, and spatial*. *Digital Discovery*. doi.org/10.1039/D5DD00193E.
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.

Technical Skills

Programming: Python, Bash, csh
Python Packages: PyTorch, PyTorch Geometric, Optuna, NumPy, CuPy, pandas, matplotlib, scikit-learn, RDKit, MolVS, Mendeleev
Modeling: AMBER, NAMD, VMD, CHARMM-GUI, AutoDock, Schrödinger, MDAnalysis, ProDy, Open Babel

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)