# 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
– Antiviral and neuropsychiatric drug discovery

## Education

**Ph.D. Candidate in Chemistry**

**GPA: 3.75**, 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 effects 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–)

**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. doi.org/10.1021/acs.jcim.5c02059.
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, MoIVS, 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)