Jose Antonio Siguenza

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Education

University of California, Berkeley **2024**

Summer Sessions (GPA 3.15)
CS61A: The Structure & Interpretation of Computer Programs
CS61BL: Data Structures and Algorithms

Escuela Superior Politecnica del Litoral (ESPOL) **2018 - 2023**

B.Sc. Chemical Engineering, (GPA: 7.95/10.00 ~ 3.44/4.00)
Thesis: Exergoeconomic optimization of a batch reactor for the production of biodiesel from used palm oil
Key Courses: Programming Fundamentals, Linear Algebra, Introduction to Data Science, Mathematics Applied to Engineer

Research and Work Experience

CIDNA-ESPOL, Ecuador, Research Scientist **2023 - present**

- Predict the mechanical properties of synthesized materials using computer vision.
- Conducted molecular simulations of protein–ligand interactions and co-authored resulting scientific publications.
- Evaluated triazole derivatives as potential cancer inhibitors using molecular docking and dynamics.

Deep Forest Sciences, Los Angeles, Computational Scientist & Research **2023 - present**

- Built and evaluated deep learning methods for genomic variant calling, equivariant geometric networks, and generative models applied to drug discovery.
- Developed a molecular docking workflow for a web app, implemented Atomic Convolutions Neural Networks for energy prediction and pose optimization, and collaborated on visualizing molecular dynamics and protein-ligand interactions.
- Contributed to open-source projects related to molecular generative models and wrote a blog on no-code large-scale molecular docking jobs.
- Enhancing equivariant capabilities for molecular data in DeepChem, specifically developing SE(3)-Transformers for molecular docking, protein-protein docking, and protein structure predictions.

Google Summer of Code, Online, Intern Student **2022**

- Contributed to DeepChem under the Open Chemistry umbrella by writing a generative model, normalizing flows, with PyTorch as the backend, along with tests and documentation to align with the organization's API.
- Authored a Jupyter notebook tutorial on using the normalizing flows model and its application in drug discovery.

ESPOL, Ecuador, Research Assistant **2021-2022**

- Applied exploratory analysis, surrogate models, and optimization algorithms using Python.
- Reviewed, automated, and generated data from simulations using ASPEN Plus.

Publications

Journal - Conference - Preprints papers

2025

J. Siguenza, H. Baykara.
"Molecular docking and dynamics simulations of 4-heteroarylidenamino-4,5-dihydro-1H-1,2,4-triazol-5-one derivatives as potential anticancer agents"
Computational Biology and Chemistry, 108657 (2025).

2025

J. Siguenza, B. Ramsundar.
"DeepChem Equivariant: SE(3)-Equivariant Support in an Open-Source Molecular Machine Learning Library"
arXiv:2510.16897 (2025).

A. Bisoi, V. Shreyas, **J. Siguenza,** B. Ramsundar. **2025**
"DeepChem-Variant: A Modular Open Source Framework for Genomic Variant Calling"
Presented at the Championing Open-Source Development in ML Workshop at ICML 2025.

Siguenza-Polo, José; Ajoy-Rendón, Karla; Mero-Benavides, Medelyne; Beltrán-Borbor, Kelly; Barcia-Quimí, Andrea; Tinoco-Caicedo, Diana L. **2025**
"Exergoeconomic Analysis and Multi-objective optimization of biodiesel production from waste cooking oil using genetic algorithm"
International Conference on Energy, Environment & Digital Transition—E2DT, 2025

V. Shreyas, **J. Siguenza**, K. Bania, B. Ramsundar. **2024**
"Open-Source Molecular Processing Pipeline for Generating Molecules"
Presented at ML4PS Workshop-NeurIPS (2024), BayLearn (2024), and MoML (2024).

J. Siguenza, H. Baykara. **2024**
"Molecular docking of triazole-based ligands with KDM5A to identify potential inhibitors."
International Workshop on Innovative Simulation for Healthcare - IWISH - I3M Conference (2024)

Under Review

C. Massay, **J. Siguenza**, M. Cornejo, and H. Baykara
"Synthesis, characterization, and mechanical property prediction of microcellulose-reinforced polyvinyl alcohol composites"
ACS Applied Polymer Materials (2025)

Awards

- Best Paper Award at International Workshop on Innovative Simulation for Healthcare IWISH - I3M Conference **2024**
- 5 Minutes Pitch Finalist at Faculty of Life Science and Mathematics at ESPOL **2023**

Academic Service

Teaching and Volunteer

- Google Summer of Code - DeepChem - Mentor **2023-2024-2025**
- Women in Data Science (WiDS) - Ecuador - Organizer **2021**

Reviewer

- International Multidisciplinary Modeling & Simulation Multiconference (I3M) **2024**
- Food Control Journal **2024**

Research Collaboration

- Generated data for "Acoustic contamination assessment during the transition between the COVID-19 restrictions and reactivation: A exploratory analysis in Guayaquil" publication." **2023**
- Wrote code scripts for "Modeling and optimization of the extraction of ylang-ylang essential oils using surrogate models from simulated data, coupled with covariance matrix adaptation evolution strategy" **2023**

Technical Skills

Software: Git, Python, Java, SQL, Scheme, Mathematica, Javascript, R, Julia.
Computer Vision : OpenCV, Torchvision.
Data Science : NumPy, SciPy, Pandas, sklearn, seaborn, Deepchem, openfe, OpenMM, MDAnalysis, biopython, pytorch geometric.
Deep Learning : PyTorch, Tensorflow, Keras, Transformers.
Databases : MySQL, MongoDB.