Jose Antonio Siguenza

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Summary

I am working in the Computational Science field, specializing in molecular docking and machine learning applications within life sciences. I hold a B.Sc. in Chemical Engineering from ESPOL, Ecuador, and have research experience in developing prediction and generative models using deep learning. My work spans fields such as molecular dynamics, protein-ligand interactions, and building generative models. I have contributed to open-source projects such as DeepChem and MDAnalysis and received recognition for my research at international conferences, including the IWISH Best Paper Award at I3M 2024. Currently, I collaborate on several peer-reviewed publications and actively contribute to research in computational drug discovery and material science.

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: 7.92/10.00)
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**

- Predict the mechanical properties of synthesized materials using computer vision. Apply molecular docking to target specific macromolecules and ligands, and publish findings in scientific papers and reports.

Deep Forest Sciences, Los Angeles, Computational Scientist **2023 - 2024**

- Developed a molecular docking workflow for a web app, implemented Atomic Convolutions Neural Networks for energy prediction and pose optimization, and collaborated on the visualization of 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.

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.

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**

Publications

Papers Under Review

Carolina Massay, **Jose Siguenza**, Mauricio Cornejo, and Haci Baykara
"Synthesis, characterization and mechanical property prediction of microcellulose-reinforced polyvinyl alcohol composites"
Materials Today Chemistry (2024)

Conferences and Peer Workshops

V Shreyas, **Jose Siguenza**, Karan Bania, and Bharath Ramsundar.
"Open-Source Molecular Processing Pipeline for Generating Molecules"

- Molecular Machine Learning Conference - NeurIPS (2024)
- BayLearn (2024)
- Molecular Machine Learning Conference - MoML (2024)

Jose Siguenza and Haci Baykara
"Molecular docking of triazole-based ligands with KDM5A to identify potential inhibitors"
International Workshop on Innovative Simulation for Healthcare - IWISH (2024)

Siguenza-Polo, José; Ajoy-Rendón, Karla; Mero-Benavides, Medelyne; Beltrán-Borbor, Kelly; Barcia-Quimí, Andrea; Tinoco-Caicedo, Diana L.
"Exergoeconomic Analysis and Multi-objective optimization of biodiesel production from waste cooking oil using genetic algorithm"
European Symposium on Computer-Aided Process Engineering - ESCAPE (2025)

Academic Service

Teaching and Volunteer

- Google Summer of Code - DeepChem - Mentor **2024**
- Google Summer of Code - Open Chemistry - Mentor **2023**
- 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.
Computer Vision : OpenCV, Torchvision.
Data Science : NumPy, SciPy, Pandas, sklearn, seaborn, Deepchem, openfe, OpenMM, MDAnalysis, biopython.
Deep Learning : PyTorch, Tensorflow, Keras, Transformers.
Databases : MySQL, MongoDB.