David Ricardo Figueroa Blanco

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Education

University of Bologna / Italian Institute of Technology (IIT) — **Genoa, Italy**
PhD in Data Science and Computation — *2020–2024*
Thesis:
Computational Approaches for Studying Enzyme Function and Protein-Ligand Interactions: From atomistic simulations to machine learning
Supervisors: Dr. Marco De Vivo

Universidad de los Andes — **Bogotá, Colombia**
MSc in Chemistry — *2018–2020*
Thesis on QM/MM Modeling of Enzymatic Reaction Mechanisms (CP2K, Gaussian)

Universidad de los Andes — **Bogotá, Colombia**
BSc in Chemistry — *2013–2018*
Graduated with Distinction (Best Thesis Presentation Award)

Research Experience

Italian Institute of Technology (IIT) — **Genoa, Italy**
Doctoral Researcher — *2020–2024*

- **AI for Drug Discovery:** Developed a 3D Convolutional Neural Network (3D-CNN) in **PyTorch** to predict high-affinity fragments for drug design. Engineered a pipeline to process ~215k PDB structures, achieving 70% top-1 accuracy.
- **Biophysical Simulation:** Conducted microsecond-scale MD simulations and Alchemical Free Energy calculations (**FEP, ATM**) using **Amber** and **OpenMM** to elucidate polymerase fidelity mechanisms.
- **Tool Development:** Created a PyMOL plugin for real-time model inference and "pocket scanning" visualization.

DeepChem — **Remote**
Google Summer of Code (GSoC) Mentor — *Summer 2024*

- Mentored a student project to enhance the DeepChem open-source library.
- Guided code architecture, conducted reviews, and ensured successful integration of new features.

Selected Publications

2024: **D. R. Figueroa Blanco**, P. Vidossich, M. De Vivo. "Correct Nucleotide Selection Is Confined at the Binding Site of Polymerase Enzymes." *J. Chem. Inf. Model.*, 64(13), 5285–5294.

2022: N. R. Elejalde-Cadena, M. García-Olave, **D. Figueroa**, et al. "Influence of Steric Effect on the Pseudo-Multicomponent Synthesis of N-Aroylmethyl-4-Arylimidazoles." *Molecules*, 27(4), 1165.

2022: A. Ballesteros-Casallas, ... **D. Figueroa**, ... M. Paulino. "Mode of action of p-quinone derivatives with trypanocidal activity studied by experimental and in silico models."

Technical Skills

Simulation: Molecular Dynamics (Amber, OpenMM, GROMACS), Free Energy Methods (FEP, TI, ATM), QM/MM (CP2K, Gaussian), Docking.

Data Science: Python (Expert), PyTorch, Scikit-learn, Pandas, NumPy, MLflow, SQL (PostgreSQL).

DevTools: Git, GitHub, Bash Scripting, Linux/HPC (SLURM), Google Gemini API, Supabase.

Languages: English (Professional), Spanish (Native), Italian (Working Proficiency).

Honors & Awards

2024: Selected Mentor, Google Summer of Code (DeepChem Organization)

2013–2018: **Beca Quiero Estudiar Escala**: Full-tuition merit scholarship (Universidad de los Andes)

2013: Gold Medal, Colombian National Chemistry Olympiad (Universidad de Antioquia)