

Nacef Guessaymi

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EDUCATION

University of Pittsburgh and Carnegie Mellon University

PhD, Molecular Biophysics and Structural Biology

- Relevant Coursework: Molecular Biophysics, Neural Signal Processing, Computational Chemistry

Aug 2018 — Current

Pittsburgh, PA

Temple University

Bachelor of Science, Biophysics

- Relevant Coursework: Thermodynamics and Statistical Mechanics, Mathematical Physics

Philadelphia, PA

Aug 2013 — May 2017

SKILLS

- **Languages:** Python, MATLAB, Rust, SQL, Bash
- **Scientific Computing:** NumPy, SciPy, Pandas, Polars, OpenMM, RDKit
- **Machine Learning:** scikit-learn, XGBoost, model inference, descriptor-based prediction
- **Infrastructure:** Linux, SLURM, Docker/Singularity, Pixi, Conda, Git
- **Quantitative Methods:** Signal Processing, Statistical Modeling, Stochastic Simulation, Data Structures & Algorithms

WORK EXPERIENCE

PhD Candidate

University of Pittsburgh

- Developed Python-based scalable computational pipelines for molecular docking, simulation, and trajectory analysis
- Designed and implemented a modular OpenMM-based software package for reproducible biomolecular energy minimization
- Performed large-scale stochastic simulations using high-performance computing environments

August 2024 — Expected Dec 2026

Pittsburgh, PA

Graduate Researcher

Carnegie Mellon University

- Built MATLAB control systems for synchronized optogenetic stimulation and electrophysiology acquisition
- Developed automated signal-processing and image-analysis pipelines for neural probe characterization
- Designed quantitative workflows for analyzing insertion-force mechanics in neural interfaces

Jan 2022 — Aug 2024

Pittsburgh, PA

Scientist II

Astrazeneca (Eurofins PSS)

- Performed high-throughput quantitative analysis and validation of biologic therapeutic assays under GMP standards
- Processed and analyzed large experimental datasets for accelerated COVID-19 therapeutic programs

Jan 2021 — Jan 2022

Gaithersburg, MD

Graduate Researcher

Carnegie Mellon University

- Extracted motion features from live-cell microscopy using MATLAB image tracking
- Extracted and analyzed cellular motion features to characterize force-dependent responses under cytoskeletal perturbations

Jun 2019 — Jan 2021

Pittsburgh, PA

Undergraduate Researcher

Temple University

- Quantified single-molecule motion from live-cell imaging using MATLAB diffusion and MSD analysis
- Reconstructed 3D spatial maps from PSF localization data using Amira

Apr 2015 — Aug 2018

Philadelphia, PA

PROJECTS

Amyloid Fibril Inhibitor Virtual Screening

- Screened a compound library against a protein target, ranking candidates by neural-network scores
- Applied clustering and dimensionality reduction (HDBSCAN, UMAP) to assess library diversity and screening convergence

2024 – Present

Stack: Python, RDKit, Gnina, Polars, scikit-learn

Amyloid Molecular Dynamics Simulation

- Large-scale stochastic simulation; optimized simulation parameters, random initial conditions, and automated topology generation
- Built checkpoint/restart tooling to resume long-running trajectories

2024 – Present

Stack: Python, AMBER (pmemd), AmberTools, MDAnalysis, Ray, SciPy

Contributor, AqSolPred-web

- Refactored an aqueous-solubility prediction model into a deployable web application for batch inference

Stack: Python, scikit-learn, XGBoost