

Nacef Guessaymi

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Education

University of Pittsburgh, PhD in Molecular Biophysics and Structural Biology – Sept 2018 – Present
Pittsburgh, PA

- Advisor: Dr. Jacob D. Durrant

Temple University, BS in Biophysics – Philadelphia, PA Sept 2013 – May 2017

- Advisor: Dr. Weidong Yang

Experience

PhD Candidate, University of Pittsburgh – Pittsburgh, PA Feb 2024 – Present

- Developed Python-based *scalable* computational pipelines for molecular docking and simulation, enabling *high-throughput* screening and *automated* trajectory analysis
- Designed and implemented a *modular* Python-based software package for biomolecular energy minimization using OpenMM, enabling *reproducible and streamlined* simulation workflows
- Performed *large-scale* structure-based virtual screening using Gnina targeting a *Staphylococcus aureus* functional fibril protein to identify modulators of amyloid assembly and biofilm formation
- Conducted molecular dynamics simulations using AMBER Force Fields to characterize conformational transitions from α -helical monomers to β -sheet fibril states
- Led a structure-based virtual screening campaign using Gnina against essential bacterial proteins in *Staphylococcus aureus* for antimicrobial discovery

Graduate Student Researcher, Carnegie Mellon University – Pittsburgh, PA Jan 2022 – Sep 2024

- Built a MATLAB-based control system for *automated* optogenetic stimulation and electrophysiological recording coordinating experimental workflow in live-animal and patch-clamp setups
- Developed Javascript-based *automated* pipelines for tissue histology analysis, *improving efficiency* and reproducibility of post-implantation assessments
- Designed MATLAB-based *automated* experimental workflows to quantify insertion forces of neural probes, enabling *systematic characterization* of mechanical interactions with tissue
- Investigated substrate-induced damage in neural probes, evaluating the impact of material properties on neural tissue integrity
- Tested Parylene-C optical waveguides for use as implantable optogenetic interfaces
 - Co-authored a peer-reviewed conference proceeding in Proceedings of SPIE (Photonics West, 2023) on implantable optogenetic waveguides
- Demonstrated the feasibility of integrated optical stimulation using flexible, biocompatible probe platforms
- Performed device characterization and validation, including optical and structural performance assessments

Bioassay Development Scientist II, Eurofins PSS – Gaithersburg, MD

Jan 2021 – Jan 2022

- Contributed to *high-throughput* sample processing and data analysis, ensuring data quality and reproducibility
- Performed bioassay development and validation for biologic therapeutics in a regulated laboratory environment
- Conducted testing and analysis of monoclonal antibody candidates, including RSV and SARS-CoV-2 programs
- Supported COVID-19 vaccine and therapeutic development efforts under accelerated timelines
 - Recognized with a Superlative Service Award for contributions to COVID-related testing efforts
- Executed cell-based and biochemical assays to assess potency, activity, and stability of drug candidates

Graduate Student Researcher, Carnegie Mellon University – Pittsburgh, PA

June 2019 – Sep 2020

- Designed and performed experiments to quantify cellular responses to mechanical stimuli
- Analyzed relationships between mechanical environment and cell fate decisions
- Investigated cellular mechanosensitivity, focusing on how mechanical forces regulate cell behavior and differentiation
 - Analyzed imaging data using an in-house computational pipeline to quantify mechanical responses
- Transfected cells with ROCK2 deletion constructs to modulate cytoskeletal contractility and investigate effects on cellular stiffness
- Studied force-dependent neural differentiation in starfish as a model system for mechanoregulation
 - Performed confocal microscopy imaging to track cellular and nuclear dynamics for force estimation

Undergraduate Researcher, Temple University – Philadelphia, PA

April 2015 – Aug 2018

- Designed and implemented a MATLAB-based mean squared displacement (MSD) *automated* analysis pipeline to quantify diffusion dynamics of FG-nups
- Characterized FG-nup dynamics and nuclear pore gating mechanisms through *integrated* imaging and computational analysis
- Performed live-cell super-resolution microscopy to investigate the dynamics of nuclear pore complex (NPC) FG-nucleoporins
- Assessed protease (3C)-mediated depletion of FG-nups to study their role in nucleocytoplasmic transport
- Co-authored multiple conference abstracts (Biophysical Journal, Molecular Biology of the Cell) and a pre-print currently under review

Publications

Small Molecule Drugs Targeting *S. aureus*

in preparation

Guessaymi N. M., Durrant J., et al

Small Molecule Inhibitors for Functional Amyloids

in submission

Guessaymi N. M., Byeon C. H., Tunc A., Rempuszewski J. J., Hansen K. H., Maldonado A. M., Urish K., Andreassen M., Durrant J., Akbey Ü

Structural and functional diversity of cerebrospinal fluid-derived α -synuclein fibrils in Parkinson's disease and multiple system atrophy

under revision

Gram H., Ollier C., Hansen K. H., Marchand T. L., Byeon C. H., Tunc A., Guessaymi N. M., Drace, T., Boggild A., Hermansholm A. K. R., Jorgensen T. J. D., Boesen T., Pintacuda G., Jensen P. H., Akbey Ü.
(Nature Communications, Submitted 10th March, 2026)

Exploring cellular gateways: unraveling the secrets of disordered proteins within live nuclear pores

Feb 2024

Yu W., Tingey M., Kelich J. M., Li Y., Yu J., Junod S. L., Jiang Z., Hansen I., Guessaymi N., Yang W.
[10.21203/rs.3.rs-3504130/v1](https://doi.org/10.21203/rs.3.rs-3504130/v1) (Nature Portfolio 2024)

In vivo optogenetic stimulation using Parylene photonic waveguides for light delivery March 2023
Reddy J. W., Jain V., **Guessaymi N.**, Malekoshoraie M. H., Chamanzar M.
[10.1117/12.2651613](#) (Proceedings of SPIE, Vol. 12366, SPIE Photonics West (2023))

Conference Abstracts & Posters

Mapping intrinsically disordered proteins in live cells by high-speed super-resolution light microscopy Feb. 2024
Yu W., Tingey M., Kelich J., Li Y., Yu J., Junod S. L., Jiang Z., Hansen I., **Guessaymi N.**, et al.
[10.1016/j.bpj.2023.11.500](#) (Biophysical Society)

Parylene Photonic Neural Probes for Minimally invasive High-resolution Optogenetic Stimulation June 2023
Guessaymi N. M., Jain V., Malekoshoraie M. H., Sarna K., Reddy J. W., Chamanzar M.
10th Annual Brain Initiative Meeting (2023)

Complete 3D mapping of FG domains for all eleven FG-Nups in living cell NPCs using super-resolution microscopy. Jan 2017
Yu J., Kelich J., Li Y., Kim J., **Guessaymi N.**, Klein M., & Yang W.
Molecular Biology of The Cell (2017)

TALKS & PRESENTATIONS

Computer-Aided Drug Design of S. Aureus Functional Fibril Inhibitors May 2026

In vivo optogenetic stimulation using Parylene photonic waveguides for light delivery Jan 2023

Selected Honors

- Brain Initiative Trainee Highlight Award (2023)
- Superlative Service (2021)

Skills

Languages: Python, Rust, MATLAB, Javascript

Computational Chemistry & Molecular Modeling: OpenMM, RDKit, AMBER, Gnina, Boltz, Chai

Electrophysiology & Signal Processing: Spike sorting (custom software development), Kilosort, Plexon, Axon, Intan

Data Science & Scientific Computing: Pandas, Polars, NumPy, SLURM

Image Analysis: OpenCV

Infrastructure & High-Performance Computing: SQL, Zarr

Research Expertise: Molecular Biophysics, Structural Biology, Computer-Aided Drug Design, Computational Pipeline Development, Electrophysiology, Image Analysis, Signal Processing, High-Performance Computing