(831)-428-9802
gjg21@pitt.edu

Gabriella Gerlach

linkedin.com/in/ggerlach
gabriellagerlach.com

Highly motivated researcher with a range of skills relevant to computational chemistry and drug discovery.

Research and Work Experience

PhD Candidate, CMU-Pitt Program in Computational Biology **Aug 2019 — July 2024 (anticipated)**

Faculty Advisor: Carlos Camacho, Associate Professor of Computational and Systems Biology Department

- Developed mechanistic understanding of the role of bacterial infection in autoimmune disorder progression in collaborative project utilizing molecular docking, molecular dynamics simulations, mouse models, patient data, and cryo-EM (in preparation)
- Discovered conserved molecular mechanism of recognition in multiple classes of SH2 domains relevant to mechanism of bacterial infection by *H. pylori* (in preparation)
- Utilized ODE simulations to provide insight to experimental collaborators on kinase modulating protein interactions
- Thesis successfully proposed Sept 2021

Computational Structural Biology Intern, Genentech **Summer 2023**

- Built and extensively tested AlphaFold based method for structure prediction of disulfide rich peptides
- Work resulted in publication at Machine Learning in Structural Biology Workshop at the 37th Conference on Neural Information Processing Systems (NeurIPS)

TECBio REU Participant, Computational and Systems Biology Department, University of Pittsburgh **Summer 2018**

Faculty Advisor: Carlos Camacho, Associate Professor of Computational and Systems Biology

- Interrogated protein interaction of p53, tumor suppressing protein, through steered molecular dynamics simulations
- Formalized work in final presentation and poster session

Undergraduate Research Assistant, Chemistry Department, Skidmore College **Jan 2017 — Jan 2019**

Faculty Advisor: K. Aurelia Ball, Assistant Professor of Chemistry

- Studied interaction of intrinsically disordered protein with SH3 domain utilizing molecular dynamics and NMR with experimental collaborators resulted in first author publication
- Developed specialized methods to compare molecular dynamics to NMR experiments and measurement of secondary structure in intrinsically disordered proteins
- Wrote successful grant proposal to expand computational power of lab

Introduction to Python Instructor, Foundation for Advanced Education in the Sciences at the NIH **Aug 2020 — Present**

- Teach 3-day introduction to Python for Bioinformatics/Computational Biology workshop to NIH students and faculty
- Generate and implement teaching material to update data analysis pipelines for many disciplines
- Instruct students both synchronously through Zoom and asynchronous through recorded lectures and assignments.
- Workshop has run 6 times to date reaching more than 85 students and receives excellent reviews

Environmental Health and Safety Technician, Chemistry Department, Skidmore College **Jan 2018 — Dec 2018**

- Evaluate and provide recommendations on the safety procedures of the laboratories on campus

Teaching Assistant, Chemistry Department, Skidmore College **Sept 2016 — Dec 2018**

- Manage set up and creation of experiments for students in general chemistry, organic chemistry, and physical chemistry
- Assist students in lab and provide feedback on assignments.

Education

PhD, Computational Biology, CMU-Pitt Program in Computational Biology, GPA: 3.68/4.00 **Aug 2019 — 2024 (anticipated)**

Bachelor of Arts, Chemistry, focus in Biochemistry, Skidmore College, GPA: 3.88/4.00 **Aug 2015 — Jan 2019**

Publications and Presentations

1. Gerlach, G. J. *et al.* A disordered encounter complex is central to the yeast Abp1p SH3 domain binding pathway. *PLoS computational biology* **16,** e1007815 (2020).
2. Gerlach, G. & Camacho, C. Sensitivity or specificity in protein interactions is independently regulated upon recognition: an SH2 case study. *Gordon Research Conference for Intrinsically Disordered Proteins* (2022).
3. Gerlach, G. & Camacho, C. Sensitivity or specificity in protein interactions is independently regulated upon recognition: an SH2 case study. *Computing Research Association Widening Participation Grad Cohort* (2022).
4. Gerlach, G. & Camacho, C. Induced fit pocket opening of MDM2 driven by anchor residue in p53. *Summer Undergraduate Research Symposium, Duquesne University* (2018).
5. Gerlach, G. & Ball, L. Characterization of Encounter Complex between ArkA and Abp1SH3. *Biophysical Society Annual Meeting* (2018).

Awards and Honors

2023 D.E. Shaw Research Graduate and Postdoctoral Women's Fellowship, Travel award - Biophysical Society Meeting,
2022 Travel awards: Computing Research Association Widening Participation Grad Cohort, Protein Society Meeting, Gordon Research Conference for Intrinsically Disordered Proteins
2021 NSF Graduate Research Fellowship Program, Honorable Mention
2019 Phi Beta Kappa Society inductee, Fayhe Award, Outstanding student in Chemistry at Skidmore College; Organic Chemistry Award, most outstanding senior in Organic Chemistry at Skidmore College

Coursework and Skills

Courses: ML	Intro to Machine Learning (CMU-10701), Scalable Machine Learning for Big Data Biology
Courses: Comp Bio	Computational Structural biology, Computational Genomics (CMU-02710), Cellular and Systems Modeling
Molecular Dynamics	Amber with AmberTools, CHARMM with NAMD, OPENMM, PyMol, VMD, Chimera
Small Molecules	Smina, Vina, Omega, openbabel, Gaussian
Programming	Python (PyTorch, Pandas, NumPy, scikit-learn, PyRosetta ect.), linux/unix environments, Git, Bash, R Google Cloud Distributed Computing, AWS

Outreach and Service to Department

Graduate Student Representative to Steering Committee **Sept 2022–present**
CMU-Pitt Program in Computational Biology

- Committee is comprised of the Directors and Associate Directors at both Universities, both program managers, and two committee appointed senior-level students
- Makes decisions on changes to the program including the student review process, curriculum, requirements, and admissions procedures

Head Graduate Student Associate to TECBio REU **Summers 2020-2022**
Department of Computational and Systems Biology, University of Pittsburgh

- Consulted program heads in transition to a fully virtual program
- Activated graduate student mentors to provide feedback in a journal club and cross school ethics forum
- Invited outside speakers from both industry and other academic institutions

Chair of CPCB Diversity Equity and Inclusion Committee **July 2020-September 2021**
CMU-Pitt Program in Computational Biology

- Organized virtual recruitment application assistance event focused on recruited historically excluded groups
- Increased eligibility for fee waivers in applications
- Involved graduate students in seminar series speaker recruitment with the goal of increasing the diversity of speakers