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Gabriella Gerlach

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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 — 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

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 **Aug 2020 — Present**
Foundation for Advanced Education in the Sciences at the NIH Virtual

- 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 **Jan 2018 — Dec 2018**
Skidmore College

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

Teaching Assistant **Sept 2016 — Dec 2018**
Skidmore College

- 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

2022 Travel award: Computing Research Association Widening Participation Grad Cohort, travel award: Protein Society Meeting
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, PyMol, VMD, Chimera
Small Molecules	Smina, Vina, Omega, openbabel, Gaussian
Programming	Python (PyTorch, Pandas, NumPy, scikit-learn, ect.), linux/unix environments, Git, Bash, 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