Julia M. Montgomery

Computational Chemist & NSF Graduate Research Fellow
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SUMMARY

Computational biochemist with a diverse background including skills in performing molecular dynamics simulations, computational biology, and general programming best practices. Driven problem solver passionate to apply new and creative ways to solve biological problems using top tier computing approaches.

EXPERIENCE

Graduate Research Assistant, Virginia Tech **2019 – Present**
Research Fellow, National Science Foundation **2021 – Present**

- Established computational protocols for polarizable molecular dynamic simulations of membranes and membrane proteins for simulation production and analysis
- Utilized OpenMM for GPU-accelerated simulations of peptides, proteins, and biological membranes
- Spearheaded team adoption of parallelized GPU and CPU tasks for simulation production and analysis, speeding up simulation time by 50%
- Parameterized epinephrine for a polarizable force field using quantum mechanics target data for fitting
- Developed and revamped internal lab wikis for molecular dynamics simulations, text-editors, and Unix used to train over 18 undergraduate and graduate students
- Mentored four students through skill building, project development, and dissemination of work
- Communicated research through talks and posters at four national conferences, three industry meetings, and five university-level events to both technical and general audiences
- Secured High-Performance Computing (HPC) resources valued over $10,000 through NSF programs
- Planned, proposed, and obtained funding for a research project via NSF GRFP Fellowship

Graduate Teaching Assistant, Virginia Tech **2020 – 2023**

- Assisted in teaching one graduate and two undergraduate courses ranging from 40 to 130 students
- Provided positive and constructive feedback on assignments and projects in a timely manner
- Developed and presented a lecture centered around hidden curriculum in computational sciences

Head Laboratory Manager, St. Joseph's University **2017 – 2019**

- Oversaw lab operations, maintained equipment, and supervised three student workers
- Balanced lab budget and chemical inventory stock, ensuring reagent availability for 10+ lab sections

Tutor, St. Joseph's University **2017 – 2019**

- Supported content and skill growth, helping over 10 students transition from probation status to graduation
- Initiated small group content-focused sessions to increase tutoring opportunities within a part-time schedule

SKILLS

- **Simulation software/analysis:** CHARMM, OpenMM, NAMD, GROMACS, LOOS, MDAnalysis
- **Enhanced sampling techniques:** PLUMED
- **Visualization:** PyMOL, VMD, Blender, ChimeraX
- **Scripting:** Python, Bash, LaTeX
- **Structural Biophysics:** MODELLER, Phyre^2, SWISS-MODEL, Molecular Docking, Rosetta
- **Virtual environments/Containers:** Conda, Docker
- **High-performance computing:** SLURM
- **Linux/Unix:** Ubuntu, Rocky Linux
- **Data visualization tools:** Grace, Matplotlib, R
- **Large-scale data analysis:** Pandas, Numpy
- **Documentation and benchmarking of code**
- **Version control:** Git, GitHub

EDUCATION

Ph.D. Biochemistry, Virginia Tech **May 2024**
B.S. in Chemistry (thesis-based); Biology Minor, St. Joseph's University **May 2019**

AVAILABLE PUBLICATIONS

1. **Montgomery, J. M.** Lemkul, J. A. 2024. *Quantifying Induced Dipole Effects in Small Molecule Permeation in a Model Phospholipid Bilayer*. **Under Review**. doi.org/10.1101/2024.03.12.584668
2. Davidson, D. S., Kraus, J. A., **Montgomery, J. M.** Lemkul, J. A. 2022. *Effects of Familial Alzheimer's Disease Mutations on the Folding Free Energy and Dipole–Dipole Interactions of the Amyloid β-Peptide*. J. Phys. Chem. B 2022, 126, 39, 7552–7566. doi.org/10.1021/acs.jpcb.2c03520

PUBLICATIONS IN PREPERATION

1. **Montgomery, J. M.**, Lemkul, J. A. *Polarizable Simulations of Two Lengths of the WALP Model Peptide*.
2. **Montgomery, J. M.**, Lemkul, J. A. *Investigating the Electrostatics Underlying Activation of the Beta-2 Adrenergic Receptor.*
3. Malewicz, K.**, Montgomery, J. M.**, McGlothlin, J. W., and Lemkul, J. A. *Understanding the Molecular Evolution of Tetrodotoxin Resistance in Sodium Channels*.

LEADERSHIP & SERVICE

Mentorship Program Chair (2023–2024), **Communications** (2022–2023), **Event Coordinator** (2019–2020)
Graduate Student Association, Virginia Tech Biochemistry

- Organized a committee to create and deploy content for a new peer mentoring program, assisting 14 first-year students transition to graduate school
- Designed updates to department web pages to encourage buy-in from current and future students & alumni

Chemistry President (2018–2019), **Biology Secretary** (2017–2018)
Biology & Chemistry Clubs, St. Joseph's University

- Established a STEM curriculum for a local preschool through monthly hands-on lessons, starting with one class, then expanding to all four classes
- Acted as a community role-model through organizing biannual blood drives and seasonal river clean-ups

HONORS & AWARDS

- Catalyzing Gender Equity at Schrödinger Symposium selected participant
- Bayer CS University Mentoring Program participant
- 4 travel grants totaling $2,500 in support
- National Science Foundation GRFP 2021 awardee
- Graduate & undergraduate Scholarships totaling ~$40,000 in support
- Brookhaven National Lab Mini-Semester selected participant
- NSF ACCESS Graduate HPC Allocation Awardee

SELECTED PRESENTATIONS (5 OF 14)

1. **Montgomery, J. M.**, Lemkul, J. A. (2024) *Investigating the Electrostatic Forces Influencing the Structure and Dynamics of the Beta-2 Adrenergic Receptor and WALP Peptide.* Poster presented at the Biophysical Society 68th Annual Meeting, Molecular Dynamics I and JUST-B Poster Sessions.
2. **Montgomery, J. M.**, Lemkul, J. A. (2023) *Investigating Membrane-Small Molecule and Membrane-Protein Interactions using Polarizable Molecular Dynamics Simulations*. Talk presented at the Virginia Tech Biochemistry Departmental Seminar Series.
3. **Montgomery, J. M.**, Lemkul, J. A. (2023) *Partitioning Free Energies and Induced Dipole Response of Small Molecules Across a POPC Membrane using Polarizable Molecular Dynamics.* Poster presented at the Catalyzing Gender Equity at Schrödinger Symposia.
4. **Montgomery, J. M.** (2023) *Using a Computer to Simulate Membranes and Membrane Proteins*. Selected Flash talk presented at the 7th Annual Virginia Tech Nutshell Games.
5. **Montgomery, J. M.**, Lemkul, J. A. (2022) *Polarization in Partitioning: Quantifying the Effects of Induced Dipoles on Amino Acid Sidechain Analogs in a POPC Membrane.* Selected Platform talk presented at the Biophysical Society 66th Annual Meeting.