

Steven Lloyd Austin, Ph.D.

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Education

Postdoctoral Scholar, Dept. of Chemistry, University of South Florida <i>Advisor: Professor H. Lee Woodcock</i>	2020-2025	Tampa, FL
Ph.D. Molecular Biophysics, Florida State University <i>Advisor: Professor Wei Yang</i>	2014-2020	Tallahassee, FL
B.A. Chemistry, University of South Florida <i>Advisor: Professor Bill J. Baker</i>	2007-2012	Tampa, FL
Minor in Biomedical Physics		

Innovation

Water Density PCA

Water is an essential component in manifesting the functionality of biomolecules. Utilizing CUDA, I coded a water density analysis that reveals the structure and dynamics of the aqueous environment enveloping simulated biomolecules. I proceeded to channel this analysis into a principal component analysis and revealed strong couplings between long-timescale protein and water structural fluctuations. This work revealed a previously unknown hydration linkage that connects an allosteric cryptic site to the enzymatic active site of TEM-1 β -lactamase.

Genetic Algorithm Transfer Entropy: GATE

Detection of casual dynamics within biomolecular simulations can provide a wealth of information concerning their functionalities. Transfer entropy has long been applied to time series to detect drive/response relationships, but can be difficult to robustly calculate for non-discrete (continuous) descriptors. Using CUDA, I developed the GATE algorithm, which utilizes a "genetic fitness" procedure to accurately compute transfer entropy from continuous signals. Utilizing GATE I was able to detect specific water fluctuations that drive protein motions among a collection of long-timescale simulations (including BPTI from D.E.Shaw Research).

eABF CHARMM Implementation

The extended adaptive biasing force method is a robust enhanced sampling approach that allows for biasing of MD simulations by various user-defined collective variables, including alchemical and geometric descriptors. The utility of the method lies in the fact that eABF simulations can be biased to align with experimentally observed distributions (SAX, NMR, etc) while accelerating exploration of dynamics accessible by the selected CV. I coded eABF within CHARMM, along with on-the-fly free energy estimators, providing input-level access to a collection of geometric CVs to explore ligand binding events and rare conformational transitions.

Research Experience

University of South Florida | Department of Chemistry | Tampa, FL | 2020-2025

Postdoctoral Researcher | Advisor: Prof. H Lee Woodcock

Outcomes: 2 published papers, contributor to funded R01 with Caren Freel-Meyers (Johns Hopkins School of Medicine) and Anton II compute time grants.

Florida State University | Institute of Molecular Biophysics | Tallahassee, FL | 2014-2020

Graduate Student Researcher | Advisor: Prof. Wei Yang

Outcomes: 2 contributed talks, 1 conference poster, 1 seminar talk

Novartis Institutes for Biomedical Research | Global Discovery Chemistry | Cambridge, MA | **2013-2014**

Open-access Separations Specialist | Supervisor: Dr. John Reilly

Outcomes: 2 published papers, 1 conference poster

Charles Stark Draper Laboratory | Bioengineering Center | Tampa, FL | **2012-2013**

Synthetic Research Assistant | Supervisor: Dr. Leila Albers

Outcomes: Successful design and synthesis of lipid-based compounds under GLP standards.

University of South Florida | Department of Chemistry | Tampa, FL | **2009-2012**

Undergraduate Researcher | Advisor: Prof. Bill Baker

Outcomes: 3 conference posters

Skills

Molecular Simulation	CHARMM Developer , Anton 2, Schrödinger, QChem, IQMol
Enhanced Sampling	Extended-system Adaptive Biasing Force , Replica Exchange, Metadynamics
Molecular Visualization	Visual Molecular Dynamics (VMD), PyMol
Machine Learning	Linear/Logistic regression, PCA, Genetic Algorithms
Programming	C+, CUDA, FORTRAN, Python, \LaTeX , MATLAB, Bash, Awk
Wet-lab techniques	Chemical Synthesis, NMR, HPLC/MPLC, MS

Research Output

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4. Wonmuk Hwang, **Steven L. Austin**, Arnaud Blondel, Eric D. Boittier, Stefan Boresch, Matthias Buck, Joshua Buckner, Amedeo Caflisch, Hao-Ting Chang, Xi Cheng, Yeol Kyo Choi, Jih-Wei Chu, Michael F. Crowley, Qiang Cui, Ana Damjanovic, Yuqing Deng, Mike Devereux, Xinqiang Ding, Michael F. Feig, Jiali Gao, David R. Glowacki, James E. II Gonzales, Mehdi Bagerhi Hamaneh, Edward D. Harder, Ryan L. Hayes, Jing Huang, Yandong Huang, Phillip S. Hudson, Wonpil Im, Shahidul M. Islam, Wei Jiang, Michael R. Jones, Silvan Käser, Fiona L. Kearns, Nathan R. Kern, Jeffery B. Klauda, Themis Lazaridis, Jinhyuk Lee, Justin A. Lemkul, Xiaorong Liu, Yun Luo, Alexander D. Jr. MacKerell, Dan T. Major, Markus Meuwly, Kwangho Nam, Lennart Nilsson, Victor Ovchinnikov, Emanuele Paci, Soohyung Park, Richard W. Pastor, Amanda R. Pittman, Carol Beth Post, Samarjeet Prasad, Jingzhi Pu, Yifei Qi, Thenmalarchelvi Rathinavelan, Daniel R. Roe, Benoit Roux, Christopher N. Rowley, Jana Shen, Andrew C. Simmonett, Alexander J. Sodt, Kai Töpfer, Meenu Upadhyay, Arjan van der Vaart, Luis Itza Vazquez-Salazar, Richard M. Venable, Luke C. Warrensford, H. Lee Woodcock, Yujin Wu, Charles L. III Brooks, Bernard R. Brooks, and Martin Karplus. CHARMM at 45: Enhancements in Accessibility, Functionality, and Speed. *The Journal of Physical Chemistry B*, **2024-09-20**
 3. Eucolona M. Toci, **Steven L. Austin**, Ananya Majumdar, H. Lee Woodcock, and Caren L. Freel Meyers. Disruption of an Active Site Network Leads to Activation of C2 α -Lactylthiamin Diphosphate on the Antibacterial Target 1-Deoxy- D -xylulose-5-phosphate Synthase. *Biochemistry*, 63(5):671–687, **2024-03-05**
 2. Felix Acheampong, John Reilly, Christopher Larbie, Matthew Spencer, Karl Gunderson, Regina Appiah-Opong, Christopher Howson, Jennifer Porier, Kellie Joyce, Valentina Jeliaskova, Sarah Voytek, Carol Ginsburg-Moraff, Stefan Thibodeaux, Jill Kublbeck, and **Steven Austin**. Methoxy-flavones identified from *Ageratum conyzoides* induce caspase -3 and -7 activations in Jurkat cells. *Journal of Medicinal Plants Research*, **2017-10**
 1. **S Austin**, D Dunstan, J Reilly, and M McKinnon. Automated Analysis of Open-Access HPLC Instrumentation Metrics. *Chromatography Today*, page 18, **2014-08-20**

Presentations & Invited Seminars

Conference Talks & Seminars

5. **Austin S.**; Wu, D.; Yang, W. (2019) **Florida Annual Meeting and Exposition (American Chemical Society: Florida Section)**, Palm Harbor, FL. Biophysical and Physical Chemistry Symposium
4. **Austin S.**; Wu, D.; Yang, W. (2019) **257th ACS National Meeting & Exposition**; Orlando, FL. Computers in Chemistry Division: Computational Studies of Water Section
3. **Austin S.**; Wu, D.; Yang, W. (2019) **257th ACS National Meeting & Exposition**; Orlando, FL. Enhanced Sampling Symposium
2. **Austin S.** (2018, 2019) **The Cell and Molecular Biology Graduate Student Association at Florida State University**; Tallahassee, FL.
1. **Austin S.**; Wu, D.; Yang, W. (2018) **Structural Biology/Biochemistry Seminar at Florida State University**; Tallahassee, FL.

Conference Posters (Presenters underlined)

8. **Austin, SL.**; Wood, HL (2024) **Annual CHARMM Meeting**; Baltimore, MD.
7. Paudel, R.; Habibzadeh, N.; **Austin, SL**; Wood, HL (2024) **Raymond N. Castle Student Research Conference**; Tampa, FL.
6. **Austin, S.**; Wu, D.; Yang, W. (2020) **259th ACS National Meeting & Exposition**; Philadelphia, PA. (Canceled due to COVID-19)
5. Okten, A.; Pinnamanteni, S.; **Austin, S.**; Yang, W. (2015) **FSU Undergraduate Research Symposium**; Tallahassee, FL.
4. **Austin, S.** (2014) **Novartis Institutes for Biomedical Research Poster Presentations**; Cambridge, MA.
3. **Austin, S**; Beau, J; Baker, B. (2011) **American Society of Pharmacognosy**; San Diego, CA.
2. **Austin, S**; Beau, J; Baker, B. (2011) **National Conference for Undergraduate Research**; Ithaca, NY.
1. **Austin, S**; Beau, J; Baker, B. (2010) **Raymond N. Castle Student Research Conference**; Tampa, FL.

Teaching Experience

General Biochemistry | *Instructor of Record* | University of South Florida | **Spring 2024**

Designed exam and course materials, proctored exams, and held office hours and recitations weekly.

General Chemistry I | *Instructor of Record* | University of South Florida | **Fall 2023**

Member of a cohort of 5 instructors covering 7 sections. Contributed to the shaping of course material in addition to the preparation and proctoring of exams.

General Chemistry II Recitation | *Teaching Assistant* | Florida State University | **Spring 2020, Fall 2015**

Prepared lesson materials and taught recitation for multiple sections (approximately 60 students). Held office hours weekly. Proctored and graded all exams.

General Biochemistry Recitation | *Teaching Assistant* | Florida State University | **Fall 2019**

Graded exams and held office hours weekly.

General Chemistry II Lab | *Teaching Assistant* | Florida State University | **Spring 2019, Summer 2017**

Supervised and assisted students in performing laboratory experiments. Graded all lab reports weekly.

Working with Dr. Stephanie Dillon (Director of Freshman Chemistry Laboratories), I designed and implemented new materials for the course, including weekly quiz questions for Canvas.

Chemistry for Liberal Studies | *Teaching Assistant* | Florida State University | **Spring 2018**

Interacted with and assisted non-major chemistry students in an immersive virtual laboratory setting powered by Second Life™.

Physical Chemistry II Recitation & Lab | *Teaching Assistant* | Florida State University | **Spring 2017**

Graded exams and held office hours weekly. Evaluated, supervised, and assisted students in performing laboratory experiments. Wrote an Excel-based analysis used by students to determine fluorescence lifetimes in a pulsed laser

experiment.

Mentorship

University of South Florida, Department of Chemistry | 2020-2024

Mentor to graduate students by contributing to the cultivation of their research, preparation of publications, as well as oral and poster presentations.

Florida State University Young Scholars Program | 2017, 2019

Mentor to high school students (3-4 students/yr) from across Florida who demonstrated academic excellence. Taught basic coding practices and introduction to molecular dynamics simulations. Students independently setup and performed simulations of enzymes and analyzed results under my guidance. Each student prepared a publication-like report and jointly created a research poster that they presented to their peers and faculty at FSU.

Foreign Exchange Mentor, Novartis Institutes for Biomedical Research | 2014

Mentor to undergraduate visiting scholars from Ghana. I taught natural products extraction techniques using state-of-the-art purification instrumentation. Our collaboration resulted in a publication and a very rewarding transfer of knowledge and ideas regarding natural products drug discovery.

Honors & Awards

NVIDIA GPU Award Finalist | Computers in Chemistry 259th ACS National Meeting | **2020**

Presentation Grant | Congress of Graduate Students | Florida State University | **2019**

Tampa Bay Seminole Club Scholarship | **2017**

Student Development Travel Grant | Institute of Molecular Biophysics | Florida State University | **2016**

Research Travel Grant | Office of Undergraduate Research | University of South Florida | **2011**

Honors College Research Travel Grant | University of South Florida | **2011**

Professional Organizations

Students for the Effective Communication of Science | 2014-2019

Institute of Molecular Biophysics, Florida State University

Vice President (2016) & Treasurer (2015)

Molecular Biophysics student organization meeting once weekly to practice presentation skills and discuss research throughout the institute. As an officer, I was responsible for organizing a yearly invited Structural Biology & Biochemistry Seminar Speaker.

The Cell and Molecular Biology Graduate Association | 2014-2019

Department Biological Science, Florida State University

Student Member

As an out-of-department member I was able to stimulate exchange of knowledge and perspective in the context of molecular functionalities from protein dynamics to cell cycles.

Professional References

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