

Accomplished PhD in Computational Biochemistry specializing in medical and science communication. Proven skills in writing and public speaking, adept at presenting complex scientific topics to varied audiences. Experienced in designing compelling presentations and educational material.

## Education

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2018 – 2023

**University of Texas at Dallas**

*PhD – Chemistry & Biochemistry*

Advisor: Dr. Hedieh Torabifard (2021 - 2023)

Dr. Steven Nielsen (2018 – 2021)

Research Area: Computational chemistry to study protein mechanisms

2013 – 2018

**Texas A&M University – Commerce**

*B.S. – Chemistry, Magna Cum Laude*

Advisor: Dr. Bukuo Ni

Research Area: Organic synthesis

## Research Experience

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01/2021 – 12/2023

**University of Texas at Dallas**, Department of Chemistry & Biochemistry

Graduate Researcher, Laboratory of Hedieh Torabifard, Ph.D.

- Performed molecular dynamics simulations on membrane and soluble proteins to understand their structure and function
- Used free energy methods such as umbrella sampling to propose transport mechanisms and compare systems
- Mentored three undergraduate students in lab training and guided research projects

01/2019 – 12/2020

Graduate Researcher, Laboratory of Steven Nielsen, Ph.D.

- Performed molecular dynamics simulations to study binding of small molecules to soluble proteins
- Collaborated with experimental biochemists to validate relative binding preferences of multiple small molecules

05/2017 – 12/2018

**Texas A&M University – Commerce**, Department of Chemistry

McNair Scholar, Undergraduate Researcher, Laboratory of Bukuo Ni, Ph.D.

- Used standard organic chemistry techniques to synthesize spirocyclic  $\delta$ -lactones by asymmetric organocatalytic reactions
- Wrote and presented detailed report of results at several conferences

## Teaching Experience

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### University of Texas at Dallas

*Graduate Teaching Assistant, Department of Chemistry & Biochemistry*

Classical Simulations for Biological and Condensed Systems (Spring 2023)

- Assisted graduate and undergraduate students with the practical knowledge needed to carry out computational chemistry calculations
- Held a once weekly workshop and office hours to review the lecture material before leading them through the software and techniques necessary for assignments and final projects
- Assisted in the proposal, experimental design, data collection, and final presentation of student projects

Physical Chemistry I & II (Spring 2020, Fall 2020, Spring 2021, Fall 2021, Spring 2022, Fall 2022)

- Hosted once weekly review sessions for 60-100 undergraduate students, with brief (30-40 minute) lecture covering relevant topics followed by problem-solving examples
- Graded all homework assignments, assisted in grading the midterm exams, and hosted weekly office hours

General Chemistry I & II Labs (Fall 2018, Spring 2019, Fall 2019)

- Each semester, supervised three lab sections with 25-30 students in each
- Hosted workshop before each experiment to cover appropriate lecture material and prepare students by covering necessary technical and safety details
- Graded workshop calculations and weekly lab reports for all students
- Established an optional Excel workshop each semester after noticing frequent student struggles in plotting and analyzing data

### Texas A&M University – Commerce

*Undergraduate Teaching Assistant, University College*

First Year Mentoring (Fall 2017)

- Taught once weekly course for 25 first-year undergraduate students to cover topics and skills related to academic success
- Served as a liaison between the students and the campus at large, helping them to find resources, and connecting with different on-campus offices and departments

Signature Course: The Quest for Happiness (Spring 2018)

- Evaluated students' assignments and in-class participation as they analyzed Aristotle's Nicomachean Ethics
- Assisted students in preparing an end-of-semester presentation to the entire freshman student body about a real-world example of concepts covered in class

## Awards & Accolades

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1. Commencement Speaker, Natural Sciences & Mathematics, UTD (2023)
2. ASBMB Advocacy Training Program Delegate (2023)
3. NVIDIA GPU Award Best Poster Finalist, ACS National Meeting (2023)
4. Outstanding Graduate Teaching Assistant, UTD Department of Chemistry & Biochemistry (2022)
5. Merck Research Award for Underrepresented Chemists of Color (2022)
6. 2<sup>nd</sup> Place Presentation, Physical/Computational Chemistry, ACS Meeting in Miniature (2022)

## Publications

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1. **Mills, K.R.**, and Torabifard, H. "Computational Approaches to Investigate F<sup>-</sup> Binding, Selectivity and Transport Across the Membrane", *Methods in Enzymology, In Preparation*
2. **Mills, K.R.**, Misra, J., and Torabifard, H. "Allosteric Modulation of YAP/TAZ-TEAD Interaction by Palmitoylation and Small Molecule Inhibitors", *BioRxiv*, DOI: 10.1101/2023.10.24.563887
3. **Mills, K.R.**, and Torabifard, H. "Uncovering the Mechanism of the Proton-Coupled Fluoride Transport in the CLC<sup>F</sup> Antiporter", *J. Chem. Inf. Model.*, 2023, 63, 8, 2445–2455, DOI: 10.1021/acs.jcim.2c01228
4. **Mills, K.R.**, Baglia, R.A., Mitra, K., Tutol, J.N., Ball, D., Page, K.M., Kallu, J., Gottipolu, S., D'Arcy, S., Nielsen, S.O., and Dodani, S.C.. "An activity-based fluorescent sensor for the detection of the phenol sulfotransferase SULT1A1 in living cells", *RSC Chem. Biol.*, 2021, 2, 830-834, DOI: 10.1039/D0CB00231C  
*\* This article is part of the themed collections: Analytical methods in chemical biology and RSC Chemical Biology Editors' Choice*
5. Graham, R.L., **Mills, K.R.**, Headley, A.D. and Ni, B.. "Asymmetric Synthesis of Spirooxindole Lactones by Ammonium-tethered Chiral Organocatalysts catalyzed Michael Addition/Cyclization of 3-hydroxyoxindoles with  $\alpha$ ,  $\beta$ -unsaturated Aldehydes", *Cur. Catal.*, 2023, 12, 1, 34-42, DOI: 10.2174/2211544712666230417104533.

## Presentations

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1. Oral Presentation: ACS Southwest Regional Meeting (2023) "Structural insights into YAP/TAZ-TEAD interaction and its regulation by small molecules"
2. Poster Presentation: ACS National Meeting (2023) "Exploring the YAP/TAZ-TEAD protein interaction and its modulation by small molecules"  
*\* This poster was one of three finalists for the NVIDIA GPU Award for best poster*
3. Oral Presentation: ACS Southwest Regional Meeting (2022) "Computational Study of a YAP/TAZ-TEAD Inhibitor"
4. Poster Presentation: UTD Research Day (2022) "Uncovering Mechanism of Transport in CLC<sup>F</sup> Protein"
5. Oral Presentation: 263<sup>rd</sup> ACS National Meeting (2022) "Investigation of coupled proton transport in CLC<sup>F</sup> F<sup>-</sup>/H<sup>+</sup> Antiporter"
6. Oral Presentation: ACS DFW Meeting in Miniature (2022) "Molecular Dynamics Study of the Proton-Coupled Fluoride Transport in the CLC<sup>F</sup> F<sup>-</sup>/H<sup>+</sup> Antiporter"  
*\* This presentation won 2<sup>nd</sup> place in the Physical/Computational section for best presentation*
7. Oral Presentation: ACS Southwest Regional Meeting (2021) "Computational Study of CLC<sup>F</sup> F<sup>-</sup>/H<sup>+</sup> Antiporter Protein"
8. Oral Presentation: 255<sup>th</sup> ACS National Meeting (2018) "Diarylpyrrolinol silyl ether as organocatalyst for asymmetric cycloaddition of  $\alpha,\beta$ -unsaturated aldehydes to 3-hydroxyoxindoles to produce spirocyclic  $\delta$ -lactones in aqueous media"
9. Oral Presentation: Texas National McNair Research Conference (2018) "Synthesis of spirocyclic  $\delta$ -lactones by asymmetric organocatalytic reactions"
10. Poster Presentation: 14<sup>th</sup> Annual Pathways Student Research Symposium (2017) "Synthesis of spirocyclic  $\delta$ -lactones..."
11. Poster Presentation: ACS Southwest Regional Meeting (2017) "Synthesis of spirocyclic  $\delta$ -lactones..."
12. Oral Presentation: TRiO McNair Scholars Showcase (2017) "Synthesis of spirocyclic  $\delta$ -lactones..."
13. Oral Presentation: Gulf Coast Student Success Conference (2016) "Teaching Scientific Writing, Even as a Non-STEM Peer Educator"

# Leadership & Service

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2022 – 2023

## Grants & Communications Director

*Science Mentorship Institute, 501(c)(3)*

- Setting up organizational infrastructure for a nonprofit organization dedicated to helping underprivileged students from around the world gain experience and mentorship in scientific research
- Creating Standard Operation Procedure for finding, accurately describing, and applying for funding opportunities
- Aiding in efforts to improve the diversity in staff and students, and highlighting this information in recruiting efforts
- Designing and implementing marketing and branding strategies to aid in recruitment and fundraising efforts

2022 – 2023

## President

*Chemistry Graduate Student Association, University of Texas at Dallas*

- Expanding the orientation events aimed at the incoming PhD students by incorporating additional social events, talks with current graduate students and faculty, and campus tours.
- Promoting diverse voices and viewpoints within the organization
- Performing and organizing several outreach talks and events:
  - National Chemistry Week 2022 with ACS DFW: performed chemistry demonstrations for hundreds of school-age children
  - Young Women's Preparatory Network, STEAM Explorers Camp, gave 30 minute talk to young girls about my career and how they can get involved in science
  - Sat on graduate student panel for several TRiO program visits to UTD from nearby schools including University of Louisiana – Lafayette, Texas A&M University Texarkana, Texas Women's University, Texas A&M University – Commerce

2021-2022

## Vice President

*Chemistry Graduate Student Association, University of Texas at Dallas*

- Helped to restart the organization after it had shut down during the pandemic.
- Organized a series of flash talks by graduate students and faculty members to introduce first year PhD students to the different research labs and on-campus resources.
- Aided in the campus-wide mercury thermometer exchange to remove unnecessary hazardous materials from research and teaching labs.
- Helped organize and moderate the ACS DFW Meeting in Miniature, a local meeting where chemistry students from around north Texas can present their research and meet students from other universities.
- Performed and organized several outreach talks and events:
  - National Chemistry Week 2021 with ACS DFW: performed chemistry demonstrations for hundreds of school-age children
  - GSA Diversity Lunch Series: School of Natural Sciences & Math panelist
  - Westwood Junior High "Ed-Talks": gave a 45 minute presentation to students about my research and career
  - Boy Scouts of America, Chemistry Merit Badge, gave a 15 minute presentation about my research

2018-2019

**First Year Liaison**

*Chemistry Graduate Student Association, University of Texas at Dallas*

- Brought attention to issues the first-year PhD students were facing and organized a “Qualifying Exam Q&A Session” and “Wellness Focus Group”

2015-2018

**Chemistry & Physics Tutor**

*Academic Success Center, Texas A&M University – Commerce*

- Taught students in both one-on-one and group settings concepts of introductory chemistry and physics
- Worked with professors to improve mandatory student workshops
- Attended and presented at Student Success conference to improve communication skills in STEM student