

Jonathan Zajac | Ph.D. Candidate | zajac028@umn.edu
Department of Chemistry | University of Minnesota, Minneapolis, MN 55455

Education

Ph.D.	University of Minnesota, Minneapolis, MN	2026 (est.)	Chemistry
M.S.	University of Minnesota, Minneapolis, MN	2023	Chemistry
B.S.	University of Wisconsin, Eau Claire, WI	2020	Biochemistry, <i>Major</i> Neuroscience, <i>Minor</i>

Research Experience

- 2021 - **Research Assistant, University of Minnesota - Twin Cities, Dept. of Chemistry**
Advisor - Sapna Sarupria
- Established a concentration-dependent “flipping” mechanism of arginine on hydrophobic interactions from a direct to indirect stabilizer.
 - Identified molecular determinants for co-excipient synergy related to hydrophobic polymer folding in binary amino acid solutions.
 - Developed a computationally-efficient simulation method for investigating virus-solvent interactions at atomistic resolution.
 - Demonstrated a unifying framework for excipient effects on the temperature dependence of protein folding/unfolding through shape complementarity.
 - Provided mechanistic insights through molecular simulations on novel agonists/antagonists targeting melanocortin receptors.
 - Actively participated in interdisciplinary collaborations spanning chemistry, chemical engineering, medicinal chemistry, and computer science.
- 2019 - 2020 **Research Apprentice, University of Wisconsin - Eau Claire, Dept. of Psychology**
Advisor - David Jewett
- Identified and assessed individual differences in stimulus control among rats trained to discriminate between naltrexone and saline.
 - Learned ethical and proper animal care and use in compliance with the Institutional Animal Care and Use Committee.
- 2017 - 2019 **Research Assistant, University of Wisconsin - Eau Claire, Dept. of Chemistry**
Advisor - Sudeep Bhattacharyay
- Performed hybrid quantum mechanical/molecular mechanical simulations to assess ligand binding, protein function, and dynamics.
 - Developed methods to identify optimal binding orientations for inhibitors of NAD(P)H:quinone oxidoreductases using geometric and energetic methods.
 - Utilized computational tools to determine the effects of mutation on the flexibility and stability of prolyl-tRNA synthetase.

Teaching Experience

- 2024 **Research Mentor**
- Led a team of 6 aspiring researchers in the design and execution of a computational project on *de novo* protein design and engineering.
 - Group composition included 1 master's student, 2 undergraduate students, and 3 high school students, spanning 5 different institutions.
- 2021 - 2022 **Teaching Assistant, UMN Department of Chemistry**
- Lectured and oversaw two general chemistry labs, each comprised of 26 undergraduate students.
 - Held office hours and aided in the design of course materials for thermodynamics.
- 2020 **Tutor, University of Wisconsin - Eau Claire, Dept. of Chemistry**
- Tutoring for general chemistry, organic chemistry, and biochemistry courses.

- 2020 **Academic Apprenticeship, University of Wisconsin - Eau Claire, Dept. of Psychology**
- Teaching assistant for behavioral and clinical neuroscience as well as psychopharmacology courses.

Honors, Awards, and Accomplishments

- 2025 **Graduate Student Award in Computational Molecular Science and Engineering (CoMSEF)**, for excellence in research by graduate students and significant contributions to research in computational molecular science and engineering. Recognized at the AIChE 2025 Annual Meeting.
- 2025 **Doctoral Dissertation Fellowship**, awarded a \$25,000 stipend, tuition stipend, and \$1,000 travel award. Awarded out of 195 doctoral candidate applicants at the University of Minnesota.
- 2025 **NSF Maximize ACCESS Grant**, awarded 14,000,000 CPU hours for simulations towards the design of stable virus and virus-like particle formulations.
- 2025 **i-CoMSE Travel Award**, awarded a \$500 travel award to attend the 10th i-CoMSE workshop on QM/MM and AIMD, hosted at Oklahoma State University.
- 2024 **NSF ACCESS Grant**, awarded 3,000,000 CPU hours for the development of a novel computational approach for *de novo* enzyme design.
- 2024 **NSF ACCESS Grant**, awarded 3,000,000 CPU hours for simulations towards the design of stable virus formulations.
- 2024 **Equity Certificate Hosted Online (ECHO)**, Office for Equity and Diversity (OED), University of Minnesota - Twin Cities
- 2024 **Grand Prize** (\$2000 Travel Award), Research Computing Exhibition, University of Minnesota - Twin Cities
- 2023 **NSF ACCESS Grant**, awarded 400,000 CPU hours for the development of a novel approach for atomistic capsid simulations.
- 2023 **Top Poster** (\$1000 Travel Award), Research Computing Exhibition, University of Minnesota - Twin Cities
- 2021 **Thank a Teacher Certificate**, received Fall 2021 for Outstanding Teaching Assistant through the Center for Educational Innovation.
- 2020 **Departmental Honors**, Dept. of Chemistry, University of Wisconsin - Eau Claire
- 2016 **Honors Scholarship**, University of Wisconsin - Eau Claire

Publications

Peer-Reviewed Journal Articles

1. **J. W. P. Zajac**, P. Muralikrishnan, C. L. Heldt, S. L. Perry, S. Sarupria, "Towards Stable Biologics: Understanding Co-Excipient Effects on Hydrophobic Interactions and Solvent Network Integrity", *Molecular Systems Design & Engineering*, 2025, 10, 432-446. doi: 10.1039/D4ME00201F (**Selected for front cover**)
2. **J. W. P. Zajac**, P. Muralikrishnan, I. Tohidian, X. Zeng, C. L. Heldt, S. L. Perry, S. Sarupria, "Flipping Out: Role of Arginine in Hydrophobic Polymer Collapse". *Chemical Science*, 2025, 16, 6780-6792. doi: 10.1039/d4sc08672d
3. P. Muralikrishnan, **J. W. P. Zajac**, C. L. Heldt, S. L. Perry, S. Sarupria, "Thermodynamic Basis of Sugar-Dependent Polymer Stabilization: Informing Biologic Formulation Design", *Journal of Physical Chemistry B*, 2025. doi: 10.1021/acs.jpccb.5c06203
4. N. Weirath, **J. W. P. Zajac**, H. Donow, T. Lavoie, C. Pinilla, R. Santos, R. Prajapati, R. Speth, M. Ericson, S. Sarupria, M. Giulanotti, C. Haskell-Luevano, "N-branched tri-cyclic guanidines as novel

melanocortin-3 receptor agonists and melanocortin-4 receptor antagonists". Journal of Medicinal Chemistry, 2025, 68, 2504-2527. doi: 10.1021/acs.jmedchem.4c01556

5. S. Dasetty, **J. W. P. Zajac**, and S. Sarupria, "Exploitation of active site flexibility-low temperature activity relation for engineering broad range temperature active enzymes", Molecular Systems Design and Engineering (Emerging Investigator series) 2023, 8, 1355-1370. doi: 10.1039/D3ME00013C (**Selected for front cover**) (**Nominated for best paper award**)
6. S. Suhail, **J. W. P. Zajac**, C. Fossum, H. Lowater, C. McCracken, N. Severson, B. Laatsch, A. Narkiewicz-Jodko, B. Johnson, J. Liebau, S. Bhattacharyya, S. Hati, "Role of Oxidative Stress on SARS-CoV (SARS) and SARS-CoV-2 (COVID-19) Infection: A Review", Protein Journal, 2020, 39(6), 644-656. doi: 10.1007/s10930-020-09935-8
7. **J. W. P. Zajac**, H. Anderson, L. Adams, D. Wangmo, S. Suhail, A. Almen, L. Berns, B. Coerber, L. Dawson, A. Hunger, J. Jehn., J. Johnson, N. Plack, S. Strasser, M. Williams, S. Bhattacharyya, S. Hati, "Effects of Distal Mutations on Prolyl-Adenylate Formation of Escherichia coli Prolyl-tRNA Synthetase", Protein Journal, 2020 39(5), 542-553. doi: 10.1007/s10930-020-09910-3

Preprints and Manuscripts in Preparation

8. **J. W. P. Zajac**, I. Tohidian, P. Muralikrishnan, S. L. Perry, C. L. Heldt, S. Sarupria. "Cracking the Capsid Code: A Computationally-Feasible Approach for Investigating Virus-Excipient Interactions in Biologics Design", bioRxiv, 2025. doi: 10.1101/2025.09.04.674344 [Manuscript in revision, submitted to the Journal of Chemical Theory and Computation]
9. **J. W. P. Zajac**, P. Muralikrishnan, S. L. Perry, C. L. Heldt, S. Sarupria. "Protein-Solvent Shape Complementarity as a Unifying Phenomenon in Excipient-Driven Formulation Stability" [Manuscript in preparation]
10. I. Tohidian, X. Zeng, **J. W. P. Zajac**, R. Chaudhari, S. Sarupria, S. Perry, C. L. Heldt. "Mechanistic Understanding of the Effect of Excipients on the Thermal Stability of Biological Molecules" [Manuscript in review, submitted to Molecular Pharmaceutics]
11. X. Zeng, **J. W. P. Zajac**, A. Sathyavageeswaran, C. L. Heldt, S. Sarupria, S. L. Perry. "Exploring the Mutual Effects of Excipient and Proteins in Complex Coacervation" [Manuscript in preparation]

Presentations, Posters, and Exhibitions

Contributed Papers Presented at Professional Meetings and Conferences

1. **J. W. P. Zajac**, P. Muralikrishnan, I. Tohidian, X. Zeng, S. Heldt, S. Perry, S. Sarupria, "Blueprinting Future-Proof Vaccines: Enhancing Formulation Stability through Molecular Simulations and Network Theory", November 2026, poster presented at American Institute of Chemical Engineers (AIChE) 2025 Annual Meeting, Boston, MA.
2. **J. W. P. Zajac**, P. Muralikrishnan, C. Heldt, S. Perry, S. Sarupria, "Probing Excipient-Driven Stability in Vaccines via Molecular Dynamics Simulations", June 2025, oral presentation at the 6th Modeling Workshop, hosted by GSK in Collegeville, PA.
3. **J. W. P. Zajac**, P. Muralikrishnan, C. Heldt, S. Perry, S. Sarupria, "Excipient architects: Redesigning solvent networks for improved protein temperature stability in liquid formulations", Mar. 2025, oral presentation at American Chemical Society annual meeting in San Diego, CA.
4. **J. W. P. Zajac**, P. Muralikrishnan, S. Sarupria, "Insights Into Excipient-Driven Stabilization of Viral Capsid Fragments Using Molecular Simulations", June 2024, oral presentation at American Society of Virology 2024 annual meeting in Columbus, OH.
5. **J. W. P. Zajac**, P. Muralikrishnan, S. Sarupria, "Designing Protein Stabilizers: Small Molecule Effects on Protein Folding are Driven by Direct Interactions and Solvent Rearrangement", Mar. 2024, oral presentation at American Physical Society annual meeting in Minneapolis, MN.

Posters and Exhibitions

6. **J. W. P. Zajac**, P. Muralikrishnan, S. Sarupria, "Navigating Complex Design Space in Modeling Temperature-Stable Therapeutics", Oct. 2024, poster presented at the NIH Chemical-Biology Interface Training Grant Symposium, University of Minnesota.
7. **J. W. P. Zajac**, S. Sarupria, "Balancing Excipient Mechanisms in the Design of Temperature-Stable Biologics", June 2024, oral presentation at the 2024 Graduate Student Research Symposium, University of Minnesota.
8. **J. W. P. Zajac**, P. Muralikrishnan, S. Sarupria, "Navigating Complex Design Space in Modeling Temperature-Stable Therapeutics", May 2024, poster presented at the Minnesota Supercomputing Institute / Research Computing Exhibition, University of Minnesota. **(Awarded grand prize)**
9. **J. W. P. Zajac**, P. Muralikrishnan, S. Sarupria, "Investigating the Effects of Arginine on Hydrophobic Interactions: Insights Towards Temperature-Stable Vaccine Design", May 2023, poster presented at the Minnesota Supercomputing Institute / Research Computing Exhibition, University of Minnesota. **(Awarded travel award)**
10. **J. W. P. Zajac**, P. Muralikrishnan, S. Sarupria, "Investigating the Effects of Arginine on Hydrophobic Interactions: Insights Towards Temperature-Stable Vaccine Design", May 2023, poster presented at the NIH Chemical-Biology Interface Training Grant Symposium, University of Minnesota.
11. **J. W. P. Zajac**, P. Muralikrishnan, C. Heldt, S. Perry, S. Sarupria, "Towards Machine Learning-Enabled Discovery of Thermostable Vaccines", Mar. 2023, poster presented at the Peter O. Stahl Advanced Design Forum, University of Minnesota.
12. **J. W. P. Zajac**, A. Vigil, S. Petit, E. Lucas, D. Jewett, "Stimulus Control Differences in Rats Given Chronic Sucrose Access and Trained to Discriminate Between Naltrexone and Saline", 2020, oral presentation at the Neuroscience Undergraduate Research Virtual Symposium (NURVS).
13. **J. W. P. Zajac**, A. Vigil, S. Petit, E. Lucas, D. Jewett, "Individual Differences in Stimulus Control Among Rats Trained to Discriminate Between Naltrexone and Saline", 2020, oral presentation at MidBrains Midwest Regional Neuroscience Conference, hosted by Augustana College.
14. **J. W. P. Zajac**, H. Stutt, H. Dorn, A. Vigil, A. Petrey, S. Petit, M. Marek, D. Jewett, "Individual Differences in Stimulus Control in Rats with Chronic-Intermittent Sucrose Access Trained to Discriminate Between Naltrexone and Saline", 2020, Abstract, FASEB Journal, 34(51). doi: 10.1096/fasebj.2020.34.s1.04224
15. **J. W. P. Zajac**, H. Stutt, H. Dorn, A. Petrey, C. Herzberg, M. Marek, D. Jewett, "Are Naltrexone's Discriminative Stimulus Effects Mediated by Kappa-Opioid Receptors in Rats with Chronic, Intermittent Sucrose Access?", 2019, poster presented at the annual Society for Neuroscience conference in Chicago, IL.
16. **J. W. P. Zajac**, N. Fruit, E. Schulz, O. Vile, H. Stutt, H. Dorn, D. Jewett, "Effects of the Kappa Agonist U69,593 on Naltrexone's Discriminative Stimulus Effect in Subjects Given Chronic, Intermittent Sucrose Access", 2019, poster presented at Celebration of Excellence in Research + Creativity (CERCA) at the University of Wisconsin - Eau Claire.
17. **J. W. P. Zajac**, S. Bhattacharyay, "Docking and Energetic Studies of Quinones and Other Aromatic Ligands in Quinone Reductases", 2018, poster presented at the annual Molecular Education and Research Consortium in Undergraduate Computational Chemistry (MERCURY) at Furman University in Greenville, SC.
18. **J. W. P. Zajac**, S. Bhattacharyay, "Calculation of Binding Free Energies of NAD(P)H:Quinone Oxidoreductase 1 Inhibitors", 2018, poster presented at Celebration of Excellence in Research + Creativity (CERCA) at the University of Wisconsin - Eau Claire.