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EDUCATION

Yale University, New Haven, CT

May 2022

Ph.D., Molecular Biophysics and Biochemistry

Integrated Program in Physical Engineering Biology

University of Wisconsin-Eau Claire, Eau Claire, WI

B.S., Biochemistry/Molecular Biology

May 2017

RESEARCH

Postdoctoral Research, Massachusetts Institute Of Technology

2022-Present

Advisor: Dr. Heather Kulik, Department of Chemical Engineering

Mechanistic and High-Throughput Studies of Metalloenzymes and Supramolecular Catalysts **Graduate Research, Yale University**2018-2022

Advisor: Dr. Sharon Hammes-Schiffer, Department of Chemistry

Proton-Coupled Electron Transfer Reactions in Biological Systems

Undergraduate Research, University of Wisconsin-Eau Claire

2014-2017

Advisor: Dr. Sudeep Bhattacharyay, Department of Chemistry

Redox Chemistry and Protein Dynamics in Flavoenzymes

PUBLICATIONS

- **16.** Nilsen-Moe, A.; **Reinhardt, C.R.**; Huang, P.; Agarwala, H.; Lopes, R.; Lasagna, M.; Glover, S.; Hammes-Schiffer, S.; Tommos, C.; Hammarström, L. Switching the Proton-Coupled Electron Transfer Mechanism for Non-Canonical Tyrosine Residues in a de novo Protein. *Chem. Sci.* **2024**, 15, 3957-3970.
- **15.** Edholm, F.; Nandy, A.; **Reinhardt, C.R.**; Kastner, D.W.; Kulik, H.J. Protein3D: Enabling Analysis and Extraction of Metal-Containing Sites from the Protein Data Bank with *molSimplify*. *J. Comput. Chem.* **2023**, 1.
- **14.** Zhong, J.; **Reinhardt, C.R.**; Hammes-Schiffer, S., Direct Proton-Coupled Electron Transfer between Interfacial Tyrosines in Ribonucleotide Reductase. *J. Am. Chem. Soc.* **2023**, 145, 4784-4790.
- **13.** Shipps, C.; Thrush, K.L., **Reinhardt, C.R.**; Siwiecki, S.A.; Claydon, J.L.; Noble, D.B.; O'Hern, C.S. Student-led workshop strengthens perceived discussion skills and community in an interdisciplinary graduate program. *FASEB BioAdvances* **2022**; 00: 1-12.
- **12. Reinhardt,** C.R*.; Konstantinovsky, D*.; Soudackov, A.V.; Hammes-Schiffer, S. Kinetic Model for Reversible Radical Transfer in Ribonucleotide Reductase. *Proc. Natl. Acad. Sci. USA* **2022**, 119, e2202022119.
- **11.** Zhong, J.; **Reinhardt, C. R**.; Hammes-Schiffer, S., Role of Water in Proton-Coupled Electron Transfer between Tyrosine and Cysteine in Ribonucleotide Reductase. *J. Am. Chem. Soc.* **2022**, 144, 7208-7214.
- **10. Reinhardt, C. R.;** Sayfutyarova, E.R.; Zhong, J.; Hammes-Schiffer, S., Glutamate Mediates Proton-Coupled Electron Transfer Between Tyrosines 730 and 731 in *Escherichia coli* Ribonucleotide Reductase. *J. Am. Chem. Soc.* **2021,** 143, 6054-6059.

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- **9. Reinhardt, C. R.;** Sequeira, R.; Tommos, C.; Hammes-Schiffer, S., Computing Proton-Coupled Redox Potentials of Fluorotyrosines in a Protein Environment. *J. Phys. Chem. B* **2021**, 125, 128-136.
- **8.** Hu, H.; Weinzetl, M.; Shulgina, I.; Weeks, K.; Fossum, C.; Adams, L.; **Reinhardt, C.R.**; Musier-Forsyth, K.; Bhattacharyya, S.; Hati, S., Editing Domain Motions Preorganize the Synthetic Active Sites of Prolyl-tRNA Synthetases. *ACS Catal.* **2020**, 10, 10229-10242. **7.** Freeze, J.G.; Martin, J.M.; Fitzgerald, P.; Jakiela, D.; **Reinhardt, C.R.**; and Newton, A. S.; Orchestrating a Highly Interactive Virtual Student Research Symposium. *J. Chem. Educ.* **2020**, 97, 2773–2778.
- **6. Reinhardt, C.R.;** Li, P.; Kang, K.; Stubbe, J.; Drennan, C.L.; Hammes-Schiffer, S. Conformational Motions and Water Structure at the α/β Interface in *E. Coli* Ribonucleotide Reductase. *J. Am. Chem. Soc.* **2020,** 142, 13768–13778.
- **5.** Nilsen-Moe, A.; **Reinhardt, C.R.**; Glover, S.D.; Liang, L.; Hammes-Schiffer, S.; Hammarström., L.; Tommos, C. Proton-Coupled Electron Transfer from Tyrosine in the Interior of a de novo Protein: Mechanisms and Primary Proton Acceptor. *J. Am. Chem. Soc.* **2020**, 142, 11550–11559.
- **4. Reinhardt, C.R.**; Huakun, H.; Bresnahan, C.G.; Hati, S.; Bhattacharyya, S. Cyclic Changes in Active Site Polarization and Dynamics Drive the 'Ping-pong' Kinetics in NRH:Quinone Oxidoreductase 2: An Insight from QM/MM Simulations. *ACS Catal.* **2018**, 8, 12015–12029.
- **3.** Goings, J.; **Reinhardt**, C.R.; Hammes-Schiffer, S. Propensity for Proton Relay and Electrostatic Impact of Protein Reorganization in Slr1694 BLUF Photoreceptor. *J. Am. Chem. Soc.* **2018**, 140, 15241–15251.
- **2. Reinhardt, C.R.**; Jaglinski, T.C.; Kastenschmidt, A.M. et al. Insight into the Kinetics and Thermodynamics of the Hydride Transfer Reactions between Quinones and Lumiflavin: A Density Functional Theory Study. *J Mol. Model.* **2016**, 22, 199.
- **1.** Bresnahan, C. G.*; **Reinhardt, C. R.***; Bartholow, T.; Rumpel, J. P.; North, M. A.; and Bhattacharyya, S. Effect of Stacking Interactions on the Thermodynamics and Kinetics of Lumiflavin: A Study with Improved Density Functionals and Density Functional Tight-Binding Protocol. *J. Phys. Chem. A* **2015**, 119, 172–182. *Equal Contributions

SELECTED ORAL PRESENTATIONS

American Chemical Society Meeting: INORG Division, Award Symposium in Honor of Rachel Narehood-Austin. 03/2024, "Role of active site residues and the protein environment in cleavage of the amide bond by a non-heme iron containing enzyme, dimethylformamidase" (invited talk)

Bucknell University Chemistry Seminar Series, 11/2022, "How Ribonucleotide Reductase Controls the Movement of Electrons Over Time and Length Scales".

Wesleyan University Biophysical Chemistry Seminar Series, 10/2021, "Conformational Influences on Proton-Coupled Electron Transfer Reactions in Ribonucleotide Reductase." **Telluride Workshop on Proton Transfer in Biology,** 06/2021, "Glutamate Mediated Proton-Coupled Electron Transfer in *E. coli* Ribonucleotide Reductase."

American Chemical Society Meeting, 04/2021, COMP Division, "Conformational Motions and Water Networks at the α/β Interface in *E. coli* Ribonucleotide Reductase."

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Yale Chemistry Symposium, Yale University, 08/2019. "Conformational Heterogeneity of the Ordered PCET Pathway in *E. Coli* Ribonucleotide Reductase."

University Honors Thesis Defense, University of Wisconsin-Eau Claire, 05/2017. "Studies of Hydride Transfer Reactions in Quinone Reductases"

American Chemical Society Meeting: PHYS Division, Computational Chemical Dynamics Symposium in Honor of Donald Truhlar. 03/2015, "Quantum Mechanical/Molecular Mechanical Simulations of the Hydride Transfer Reactions in Quinone Reductase II"

INSTRUCTIONAL EXPERIENCE

| INSTRUCTIONAL EXPERIENCE | |
|---|------------------------|
| Postdoctoral: | |
| Kaufman Teaching Certificate Program | Spring 2023 |
| Graduate: | |
| Principles of Biochemistry Head Teaching Assistant | Fall 2019 |
| Principles of Biochemistry Teaching Assistant | Fall 2018 |
| Yale Young Global Scholars Lead Instructor | Summer 2018 & 2019 |
| Undergraduate: | |
| Biophysical Chemistry Laboratory Instructional Assistant | 2016 |
| General Chemistry II Laboratory Assistant | 2015-2016 |
| University Honors Program Freshman Seminar Instructor | 2015 |
| SELECTED AWARDS | |
| Postdoctoral (External): | |
| Arnold O. Beckman Postdoctoral Fellowship in Chemical Sciences (Rese | <i>earch</i>) 2023 |
| Graduate (External): | |
| National Science Foundation Graduate Research Fellow (Research, Outr | reach) 2019 |
| Ford Foundation Predoctoral Fellowship Honorable Mention (Research, | Outreach) 2019 |
| Graduate (Internal): | |
| Mary Ellen Jones Dissertation Prize (Molecular Biophysics & Biochemis | • / |
| Robert E. MacNab Memorial Prize (Molecular Biophysics & Biochemist | try, Best 2018 |
| Poster Presentation at Departmental Retreat) | 2010 |
| Undergraduate (External): | |
| Outstanding College Chemistry Student (Central Wisconsin Section of A | , |
| Excellence in Undergrad. Research Poster Presentation (Comp. Division | 251 st 2016 |
| National ACS Meeting) | |
| Undergraduate (Internal): | |
| Ronald E. McNair Postbaccalaureate Achievement Program (Academics | 2015-2017 |
| Diversity) | 2017 2016 |
| Dr. Jack Pladziewicz Research Scholarship (Excellence in Research) | 2015-2016 |
| COMMUNITY LEADERSHIP & SERVICE | |
| American Chemical Society-New Haven Section (ACS-NH) | 2018-2022 |

Científico Latino Graduate Student Mentorship Initiative 2019-Current Program that pairs students from underrepresented groups in STEM with mentors to guide them through the graduate school application process and 1st year of grad. school

• Secretary (2019-2022), Chemists Celebrate Earth Week Coordinator (2020,2021,2022)

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Open Labs 2017-2020

Graduate student outreach group working with K-8th graders in the New Haven School District. Volunteered 20+ hours performing science demonstrations in community events.

• Finance Chair (2018, 2019)

PROFESSIONAL SERVICE

Proposal Peer Review (1)

2024: United Kingdom Research and Innovation: Biotechnology and Biological Sciences Research Council (BBSRC)

Journal Peer Review (2)

2023: The Biophysicist, The American Journal of Undergraduate Research

STUDENTS MENTORED

GS = **Graduate Student**, **UG** = **Undergraduate Student**

MIT: Melissa Manetsch (GS), Wilson Ho (UG), Tigest Aboye (UG) Yale: Jiayun Zhong (GS), Kevin Zhu (GS), Raquel Sequiera (UG)