

## EDUCATION

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| <b>Yale University, New Haven, CT</b>                     | May 2022 |
| Ph.D., Molecular Biophysics and Biochemistry              |          |
| Integrated Program in Physical Engineering Biology        |          |
| <b>University of Wisconsin-Eau Claire, Eau Claire, WI</b> | May 2017 |
| B.S., Biochemistry/Molecular Biology                      |          |

## RESEARCH

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| <b>Postdoctoral Research, Massachusetts Institute Of Technology</b>                    | 2022-Present |
| Advisor: Dr. Heather Kulik, Department of Chemical Engineering                         |              |
| Mechanistic and High-Throughput Studies of Metalloenzymes and Supramolecular Catalysts |              |
| <b>Graduate Research, Yale University</b>  | 2018-2022    |
| Advisor: Dr. Sharon Hammes-Schiffer, Department of Chemistry                           |              |
| Proton-Coupled Electron Transfer Reactions in Biological Systems                       |              |
| <b>Undergraduate Research, University of Wisconsin-Eau Claire</b>                      | 2014-2017    |
| Advisor: Dr. Sudeep Bhattacharyay, Department of Chemistry                             |              |
| Redox Chemistry and Protein Dynamics in Flavoenzymes                                   |              |

## PUBLICATIONS

- 21.** Hendricks, L.; **Reinhardt, C.R.**; Green, T.; Kunczynski, L.; Roberts, A.J.; Miller, N.; Rafalin, N.; Kulik, H.J.; Groves, J.T.; Austin, R.N.; Alkane Monooxygenase (AlkB) is an Alkyl Fluoride Dehalogenase. *Submitted*
- 20.** Chow, M.; **Reinhardt, C.R.**; Hammes-Schiffer, S. Quantum Mechanical/Molecular Mechanical Free Energy Simulations of Ribonucleotide Reductase. *Submitted*
- 19.** **Reinhardt, C. R.**; Lee, J.; Hendricks, L.; Green, T.; Kuncyznski, L.; Roberts, A.; Miller, N.; Rafalin, N.; Kulik, H. J.; Pollock, C.; Austin, R.N. No Bridge Between Us: Two Distant Iron Ions Comprise the Active Site of Alkane Monooxygenase (AlkB). *Submitted and available on ChemRxiv.*
- 18.** Kastner, D.W.; **Reinhardt, C.R.**; Adamji, H.; Manetsch, M.T.; Román-Leshkov, Y.; Kulik, H. J. Dynamic Charge Distribution as a Key Driver of Catalytic Reactivity in an Artificial Metalloenzyme. *Posted on ChemRxiv, revising for resubmission*
- 17.** **Reinhardt, C.R.**; Manetsch, M.T.; Li, W.L.; Román-Leshkov, Y.; Head-Gordon, T.; Kulik, H. J. Computational Screening of Putative Transition Metal Complexes as Guests in a Ga<sub>4</sub>L<sub>6</sub> Nanocage. *Inorg. Chem.* **2024**, 63, 14609–14622.
- 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.* **2024**, 45, 352.

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.\***; Konstantinovskiy, 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 *E. coli* Ribonucleotide Reductase. *J. Am. Chem. Soc.* **2021**, 143, 6054-6059. Corrected: *J. Am. Chem. Soc.* **2024**
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.; Weinzel, 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  $\alpha/\beta$  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

**Free University of Tbilisi (Tbilisi, Georgia):** 07/2024 “Enzyme catalysis in silico: Using theoretical chemistry and bioinformatics to investigate enzyme mechanisms and identify conserved active sites”

**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”. (invited talk)

**Wesleyan University Biophysical Chemistry Seminar Series,** 10/2021, “Conformational Influences on Proton-Coupled Electron Transfer Reactions in Ribonucleotide Reductase.” (invited talk)

**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  $\alpha/\beta$  Interface in *E. coli* Ribonucleotide Reductase.”

**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

### 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

Summers 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 (*Research*)

2023

### Graduate (External):

National Science Foundation Graduate Research Fellow (*Research, Outreach*)

2019

## Clorice R. Reinhardt

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| Ford Foundation Predoctoral Fellowship Honorable Mention ( <i>Research, Outreach</i> )   | 2019      |
| <b>Graduate (Internal):</b>  |           |
| Mary Ellen Jones Dissertation Prize ( <i>Molecular Biophysics &amp; Biochemistry</i> )   | 2022      |
| Robert E. MacNab Memorial Prize ( <i>Molecular Biophysics &amp; Biochemistry, Best Poster Presentation at Departmental Retreat</i> ) | 2018      |
| <b>Undergraduate (External):</b>   |           |
| Outstanding College Chemistry Student ( <i>Central Wisconsin Section of ACS</i> )  | 2016      |
| Excellence in Undergrad. Research Poster Presentation ( <i>Comp. Division 251<sup>st</sup> National ACS Meeting</i> )                | 2016      |
| <b>Undergraduate (Internal):</b>   |           |
| Chair's Award-Chemistry Department Scholarship ( <i>Service to Department</i> )  | 2017      |
| Ronald E. McNair Postbaccalaureate Achievement Program ( <i>Academics, Diversity</i> )   | 2015-2017 |
| Dr. Jack Pladziewicz Research Scholarship ( <i>Excellence in Research</i> )  | 2015-2016 |
| Chemistry Mentoring Scholarship ( <i>Mentoring</i> )   | 2015-2016 |

## COMMUNITY LEADERSHIP & SERVICE

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|---|--------------|
| <b>Científico Latino Graduate Student Mentorship Initiative</b>   | 2019-Current |
| Program that pairs students from underrepresented groups in STEM with mentors to guide them through the graduate school application process and 1 <sup>st</sup> year of grad. school  |              |
| <b>American Chemical Society-New Haven Section (ACS-NH)</b>   | 2018-2022    |
| • Secretary (2019-2022), Chemists Celebrate Earth Week Coordinator (2020,2021,2022)   |              |
| <b>Open Labs</b>  | 2017-2020    |
| Graduate student outreach group working with K-8 <sup>th</sup> graders in the New Haven School District. Volunteered 20+ hours performing science demonstrations in community events. |              |
| • Finance Chair (2018, 2019)  |              |

## PROFESSIONAL SERVICE

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| <b>Proposal Peer Review (1)</b>  |
| United Kingdom Research and Innovation: Biotechnology and Biological Sciences Research Council (BBSRC) |
| <b>Journal Peer Review (3)</b>   |
| Inorganic Chemistry, The Biophysicist, The American Journal of Undergraduate Research                  |

## STUDENTS MENTORED

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

**At MIT:** Melissa Manetsch (GS), Anh Nguyen (GS), Wilson Ho (UG), Tigest Aboye (UG)

**At Yale:** Jiayun Zhong (GS), Kevin Zhu (GS), Raquel Sequiera (UG)