

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	May 2017
B.S., Biochemistry/Molecular Biology	

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

- 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.** Austin, R.N.; **Reinhardt, C.R.**; Feng, L. Alkane-oxidizing enzyme AlkB. *Accepted in Encyclopedia of Inorganic and Bioinorganic Chemistry*
- 19.** **Reinhardt, C. R.**; Lee, J.; Hendricks, L.; Green, T.; Kunczynski, 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). *J. Am. Chem. Soc.* **2025**, 147, 3, 2432–2443.
- 18.** Chow, M.; **Reinhardt, C.R.**; Hammes-Schiffer, S. Nuclear Quantum Effects in Quantum Mechanical/Molecular Mechanical Free Energy Simulations of Ribonucleotide Reductase. *J. Am. Chem. Soc.* **2024**, 146, 48, 33258–33264.
- 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 Ga₄L₆ 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 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

Bioinorganic Chemistry Graduate Research Seminar, 01/2025 “Computational Investigations of Alkane Monooxygenase B”

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 α/β 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

Ford Foundation Predoctoral Fellowship Honorable Mention (*Research, Outreach*) 2019

Clorice R. Reinhardt

Graduate (Internal):

Mary Ellen Jones Dissertation Prize (<i>Molecular Biophysics & Biochemistry</i>)	2022
Robert E. MacNab Memorial Prize (<i>Molecular Biophysics & Biochemistry, Best Poster Presentation at Departmental Retreat</i>)	2018

Undergraduate (External):

Outstanding College Chemistry Student (<i>Central Wisconsin Section of ACS</i>)	2016
Excellence in Undergrad. Research Poster Presentation (<i>Comp. Division 251st National ACS Meeting</i>)	2016

Undergraduate (Internal):

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

Cientifico 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

American Chemical Society-New Haven Section (ACS-NH) 2018-2022

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

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)

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

Journal Peer Review (5)

Journal of the American Chemical Society, Journal of Chemical Theory and Computation, Inorganic Chemistry, The Biophysicist, The American Journal of Undergraduate Research

STUDENTS MENTORED

GS = Graduate Student, UG = Undergraduate Student, VS = Visiting Student/Faculty

At MIT: Égil de Brito Sá (VS), Melissa Manetsch (GS), Anh Nguyen (GS), Wilson Ho (UG), Tigist Aboye (UG)

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