

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

20. Chow, M.; **Reinhardt, C.R.**; Hammes-Schiffer, S. Nuclear Quantum Effects in 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: EXAFS And Computations Confirm 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 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 *Escherichia coli* Ribonucleotide Reductase. *J. Am. Chem. Soc.* **2021**, 143, 6054-6059. #Correction submitted
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, #Correction submitted

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 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
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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 (<i>Research</i>)	2023
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Graduate (External):

National Science Foundation Graduate Research Fellow (<i>Research, Outreach</i>)	2019
Ford Foundation Predoctoral Fellowship Honorable Mention (<i>Research, Outreach</i>)	2019

Graduate (Internal):

Mary Ellen Jones Dissertation Prize (<i>Molecular Biophysics & Biochemistry</i>)	2022
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Clorice R. Reinhardt

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

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 1 st 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-8 th 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
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)