Clorice R. Reinhardt

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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 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. 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*

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 Monoxygenase (AlkB). *In revision*

18. Chow, M.; **Reinhardt, C.R.;** Hammes-Schiffer, S. Nuclear Quantum Effects in Quantum Mechanical/Molecular Mechanical Free Energy Simulations of Ribonucleotide Reductase. *Accepted in J. Am. Chem. Soc.*

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_4L_6 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*.; 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 *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.; 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

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

Graduate (Internal):

Mary Ellen Jones Dissertation Prize (*Molecular Biophysics & Biochemistry)* 2022

Robert E. MacNab Memorial Prize (*Molecular Biophysics & Biochemistry, Best Poster Presentation at Departmental Retreat)* 2018

Undergraduate (External):

Outstanding College Chemistry Student (*Central Wisconsin Section of ACS*) 2016

Excellence in Undergrad. Research Poster Presentation (*Comp. Division 251st National ACS Meeting*) 2016

Undergraduate (Internal):

Chair's Award-Chemistry Department Scholarship (*Service to Department*) 2017

Ronald E. McNair Postbaccalaureate Achievement Program (*Academics, Diversity*) 2015-2017

Dr. Jack Pladziewicz Research Scholarship (*Excellence in Research*) 2015-2016

Chemistry Mentoring Scholarship (*Mentoring*) 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 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 (3)

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)