DAVID W. KASTNER

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Education

Ph.D. Bioengineering	Massachusetts Institute of Technology	*Current*
B.S. Biophysics	Brigham Young University, Provo, Utah	2019
	GPA **4.0** | Honors | *Summa Cum Laude*, *Valedictorian Speech*	

Honors

Prestigious Awards

ACS Chemical Computing Group Research Excellence Award	2024
Cornell Colman Inclusive Leadership Award	2021
Alfred P. Sloan Exemplary Mentorship Award (UCEM)	2019
Elva Pedersen Jorgenson Scholarship	2019
Warren Rollins and Murdell Hull Scholarship	2019
National Hispanic Fund Scholarship (HSF)	2018
Lieutenant Governor's Community Service Award	2018
National President's Volunteer Service Award	2018
National Honor Society Phi Kappa Phi Outstanding Student Award	2018
Karl G. Maeser Scholarship	2018
University Undergraduate Research Award (URA)	2018
National Barry Goldwater Scholarship	2017
National American Chemical Society Scholars Award (ACS)	2017
Full-Ride Merit-Based Scholarship	2017

Fellowships

MIT Whitehead Fellowship	2021
Vice Chancellor's Inclusive Excellence Fellowship	2020
National Science Foundation Graduate Research Fellowship (NSF GRFP)	2019
Tolero Pharmaceuticals Fellowship	2018
Inspired Learning University Fellowship	2018
Simmons Center for Cancer Research Fellowship (SCCR)	2017

Research/Professional Experience

Massachusetts Institute of Technology (MIT) – *Cambridge, MA* Sept 2020 – Current

Co-Advisors: Dr. Forest White and Dr. Heather J. Kulik
Description: Bioengineering PhD candidate studying enzyme engineering through mechanistic insights gained through quantum mechanical calculations and molecular dynamics simulations.

Pfizer Pharmaceutical Internship – *Cambridge, MA* Sept 2023 – Jun 2024

Advisor: Dr. Zhechun Zhang
Description: Built machine learning workflows for predicting protein-protein interactions and the binding sites of molecular-glue degraders.

Huntsman Cancer Institute (HCI) – *Salt Lake City, UT* Dec 2018 – Aug 2020

Advisor: Dr. Trudy G. Oliver
Description: Full-time biologist researching small cell, adenocarcinoma, and squamous lung cancer.

National Institutes of Health (NIH) – *Bethesda, MD* Jul 2018 – Sept 2018

Advisor: Dr. Nico Tjandra
Description: Internship investigating Bax-catalyzed fibril formation implicated in apoptosis.

Dana-Farber/Harvard Cancer Center (DFCI/HCC) – *Boston, MA* Apr 2018 – Jul 2018

Advisor: Dr. Haribabu Arthanari
Description: Internship investigating methods of leveraging metabolism to isotopically label proteins.

Simmons Center for Cancer Research (SCCR) – *Salt Lake City, UT* May 2016 – Apr 2018

Advisor: Dr. Steven L. Castle
Description: Engineered a potent anticancer peptide in collaboration with *Bristol-Myers Squibb*.

Computational and Synthetic Chemistry Researcher – *Provo, UT* Aug 2014 – Aug 2017

Advisor: Dr. Steven L. Castle
Description: Computational investigation of rare peptides containing unusual non-standard residues.

Humanitarian Missionary – *Osorno, Southern Chile* Apr 2012 – Apr 2014

Supervisor: John E. Rappleye
Description: Spanish-speaking full-time humanitarian volunteer across 20 cities in the Osorno region over a two-year period (over 40 hours a week).

Front Cover Highlighted Publications (Google Scholar) (ORCID)

1. **[Front Cover]** **Kastner, D.W.**; Nandy, A.; Mehmood, R.; Kulik, H.J. Mechanistic Insights into Substrate Positioning That Distinguishes Non-heme Fe(II)/a-Ketoglutarate-Dependent Halogenases and Hydroxylases. *ACS Catal.* **2023**, 13 (4), 2489-2501. DOI: 10.1021/acscatal.2c06241.

2. **[Front Cover]** Duan, C.; Nandy, A.; Terrones, G.G.; **Kastner, D.W.**; Kulik, H.J. Active Learning Exploration of Transition-Metal Complexes to Discover Method-Insensitive and Synthetically Accessible Chromophores. *JACS Au* **2023**, 3 (2), 391-401. DOI: 10.1021/jacsau.2c00547.

3. **[Front Cover]** Del Rio Flores, A.; **Kastner, D.W.**; Du, T.; Narayanamoorthy, M.; Shen, Y.; Cai, W.; Vennelakanti, V.; Zill, N.A.; Dell, L.B.; Zhai, R.; Kulik, J.H.; Zhang, W. Probing the Mechanism of Isonitrile Formation by a Non-Heme Iron(II)-Dependent Oxidase/Decarboxylase. *JACS* **2022**, 144 (13), 5893-5901. DOI: 10.1021/jacs.1c12891.

4. **[Front Cover]** Nazemi, A.; Steeves, A.H.; **Kastner, D.W.**; Kulik, H.J. Influence of the Greater Protein Environment on the Electrostatic Potential in Metalloenzyme Active Sites: The Case of Formate Dehydrogenase. *J. Phys. Chem. B* **2022**, 126 (22), 4069-4079. DOI: 10.1021/acs.jpcb.2c02260.

5. **[Front Cover]** Lo, C.L.L.; Joaquin, D.; Moyá, D.A.; Ramos, A.; **Kastner, D.W.**; White, S.A.; Christensen, B.L.; Naglich, J.G.; Degnen, W.J.; Castle, S.L. Synthesis and Evaluation of Potent Yaku'amide A Analogs. *Chem. Sci.* **2022**, 13, 1899-1905. DOI: 10.1039/D1SSC05992K.

Other Peer-reviewed Publications

6. Del Rio Flores, A.; Zhai, R.; **Kastner, D.W.**; Seshadri, K.; Yang, S.; Matias, K.D.; Shen Y.; Cai, W.; Narayanamoorthy, M.; Do, N.B.; Xue, Z.; Marzooqi, D.A; Kulik, H.J.; Zhang, W. Enzymatic Synthesis of Azide by a Promiscuous N-nitrosylase. *Nature Chemistry*. **In press**.

7. **Kastner, D.W.**; Reinhardt, C.R.; Adamji, H.; Manetsch, M.; Roman-Leshkov, Y.; Kulik, H.J. Dynamic Charge Distribution as a Key Driver of Catalytic Reactivity in an Artificial Metalloenzyme. *ChemRxiv*. **2024**. DOI: 10.26434/chemrxiv-2024-xhlgh.

8. 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, 45 (6), 352-361. DOI: 10.1002/jcc.27242.

9. Kim, C.Y.; Mitchell, A.J.; **Kastner, D.W.**; Albright, C.E.; Michael, A.G.; Glinkerman, C.M.; Kulik, H.J.; Weng, J. Emergence of a protein exchange-based isomerization and lactonization mechanism in the plant coumarin synthase COSY. *Nat. Commun.* **2023**, 14 (597). DOI: 10.1038/s41467-023-36299-1.

10. Nandy, A.; Adamji, H.; **Kastner, D.W.**; Vennelakanti, V.; Nazemi, A.; Liu, M.; Kulik, H.J. Using Computational Chemistry to Reveal Nature's Blueprints for Single-Site Catalysis of C–H Activation. *ACS Catal.* **2022**, 12 (15), 9281-9306. DOI: 10.1021/acscatal.2c02096.

11. Nandy, A.; Terrones, G.; Arunachalam, N.; Duan, C.; Duan, C.; **Kastner, D.W.**; Kulik, H.J. MOFSimplify, Machine Learning Models with Extracted Stability Data of Three Thousand Metal-Organic Frameworks. *Nat. Sci. Data* **2022**, 9 (74). DOI: 10.1038/s41597-022-01181-0.

12. Olsen, R.R.; Ireland, A.S.; **Kastner, D.W.**; Groves, S.M.; Spainhower, K.B.; Pozo, K.; Kelenis, D.P.; Whitney, C.P.; Guthrie, M.R.; Wait, S.J.; Soltero, D.; Witt, B.L.; Quaranta, V.; Johnson, J.E.; Oliver, T.G. ASCL1 Represses a SOX9+ Neural Crest Stem-like State in Small Cell Lung Cancer. *Genes Dev.* **2021**, 37, 13-14. DOI: 10.1101/gad.348295.121.

13. Ireland, A.S.; Micinski, A.M.; **Kastner, D.W.**; Guo, B.; Wait, S.J.; Spainhower, K.B.; Conley, C.C.; Chen, O.S.; Guthrie, M.R.; Soltero, D.; Qiao, Y.; Huang, X.; Tarapcsak, S.; Devarakonda, S.; Chalishazar, M.D.; Gertz, J.; Moser, J.C.; Marth, G.; Puri, S.; Witt, B.L.; Spike, B.T.; Oliver, T.G. MYC Drives Temporal Evolution of Small Cell Lung Cancer Subtypes by Reprogramming Neuroendocrine Fate. *Cancer Cell* **2020**, *38* (1), 60-78. DOI: 10.1016/j.ccell.2020.05.001.

14. Joaquin, D.; Lee, M. A.; **Kastner, D. W.**; Singh, J.; Morrill, S. T.; Damstedt, G.; Castle, S. L. Impact of Dehydroamino Acids on the Structure and Stability of Incipient 3_{10}-Helical Peptides. *J. Org. Chem.* **2020**, *3* (85), 1601-1613. DOI: 10.1021/acs.joc.9b02747.

15. Morris, D.L.; **Kastner, D.W.**; Johnson, S.; Strub, M.; He, Y.; Bleck, C.K.; Lee, D.; Tjandra, N.; Humanin induces conformational changes in the apoptosis regulator BAX and sequesters it into fibers, preventing mitochondrial outer-membrane permeabilization. *J. Biol. Chem.* **2019**, *50* (294), 19055-19065. DOI: 10.1074/jbc.ra119.0112977.

16. Kastner, D.W. Computational Modelling of Peptides Containing Non-Standard Amino Acids *Undergraduate Honors Thesis* **2019**. *ScholarsArchive*, 61. ISSN: 2572-4479.

17. Kastner, D.W. The Ultimate Triumph of Truth. *Brigham Young University Commencement*, **2019**. URL: speeches.byu.edu.

18. Ashraf, N.M., Krishnagopal, A., Hussain, A,. **Kastner, D.W.**, Sayed, A.M., Mol Y.K., Swaminathan. K., Zeeshan, N. Engineering of serine protease for improved thermostability and catalytic activity using rational design. *Int. J. Biol. Macromol.* **2018,** 126, 229-236. DOI: 10.1016/j.ijbiomac.2018.12.218.

19. Jalan, A.; **Kastner, D.W.**; Webber, K.G. I.; Smith, M.S.; Price, J.L.; Castle, S.L. Bulky dehydroamino acids enhance proteolytic stability and folding in β-hairpin peptides. *Org. Lett.* **2017**, *19* (19), 5190-5193. DOI: 10.1021/acs.orglett.7b02455.

20. Ashraf, N.M.; Imran, K.; **Kastner, D.W.**; Ikram, K.; Mushtaq, A.; Hussain, A.; Zeeshan, N. Potential involvement of mi-RNA 574-3p in progression of prostate cancer: A bioinformatic study. *Mol. Cell. Probes* **2017**, *36*, 21-28. DOI: 10.1016/j.mcp.2017.07.002.

Submitted and In-Progress Publications

1. Torrens-Spence, P.M.; Matos, O.J.; **Kastner, D.W.**; Li, T.; Glinkerman, M.C.; Sherk, J.; Wang, Y.; Kulik, H.J. Weng, J. Mechanistic Basis for the Emergence of EPS1 as a Catalyst in Plant Salicylic Acid Biosynthesis. *Nat. Commun*. *Submitted.*

2. Kastner, D.W.; Kulik, H.J.; Zhang, Z. Evaluation of In-silico Structural Predictions of Glue-Induced Ternary Complexes with Generative Models. *ACS Med. Chem. Lett. Submitted*.

3. Kastner, D.W.; Clorice, R.R.; Kulik, H.J. Mechanistic Insights into the Reaction of the Non-Heme Iron Enzyme DMFase. *In preparation.*

4. Kastner, D.W.; Wilson, H.; Luo, W.; Clorice, R.R.; Kulik, H.J. QuantumPDB: Automatic generation of quantum mechanical cluster models for high-throughput screening of protein structures. *In preparation*.

5. Colin, Y.K.; **Kastner, D.W.**; Mitchell, J.A.; Gutierrez, M.A.; Yao, S.J.; Neumann, N.E.; Kulik, J.H.; Weng, J. Chromosomal-Level Genome Assembly of *Menispermum canadense* Sheds Light on the Evolutionary Origin of Dechloroacutamine Halogenase. *In preparation.*

Conference and Poster Presentations

1. **Kastner, D.W.**; Clorice, R.; Adamji, H.; Manetsch, M.; Kulik, H.J. Mechanistic Insights from Electronic Properties in Artificial Mini-enzymes. *ACS Spring Conference New Orleans*, **2024**. DOI: 10.1021/scimeetings.4c10442.

2. **Kastner, D.W.**; Nandy, A.; Mehmood, R.; Kulik, H.J Substrate positioning in Non-heme Fe(II)/α-ketoglutarate-dependent halogenases and hydroxylases: A computational study. *Virtual Conference on Chemistry and its Applications (VCCA)*, **2023**. Video recording.

3. **Kastner, D.W.**; Jalan, A.; Castle, S. L. Conformational ensemble calculations of proteolytically stable β-hairpins containing bulky α,β-dehydroamino acids. *American Chemical Society 254th National Meeting*, Washington D.C., **2017**.

4. **Kastner, D.W.**; and Castle, Steven L., Progress toward synthetically simplified natural anticancer peptide (2018). *Library Undergraduate Poster Competition* **2018**, *5*. ISSN: 2572-4479

5. **Kastner, D.W.**; Castle, S. L. Computational predictions β-hairpins containing bulky dehydroamino acids. *Scholars Archive* **2017**, *4*. ISSN: 2572-4479

6. **Kastner, D.W.**; Lo, C. C. L.; Castle, S. L. Progress towards a synthetically simplified anticancer peptide. *Student Research Conference (SRC)*, Provo, **2018**.

7. **Kastner, D.W.**; Jalan, A.; Castle, S. L. QM/MM analysis of proteolytically stable β-hairpins. *Student Research Conference (SRC)*, Provo, **2017**.

8. **Kastner, D.W.**; Castle, S. L. ONIOM geometry optimization of bulky dehydroamino acids in β-hairpins. *IEEE Poster Session*, Provo, **2017**.

Community Service

1. Starting in 2022, I have been a dedicated weekly volunteer as a Hispanic youth group leader, mentoring Spanish-speaking youth from across South and Central America such as El Salvador, Guatemala, Venezuela, the Dominican Republic, and Mexico.

2. Served as Executive Secretary and Sunday School teacher for a Hispanic Spanish-speaking denomination, supporting over 50 weekly participants in Cambridge area.

3. Taught a highly-rated MIT IAP course (20.S947) on 3D scientific visualization to over 20 PhD students [Promotional], with the open-source version viewed by thousands worldwide [GitHub] [Videos].

4. Actively involved as a peer-reviewer, having been invited to review and successfully completed 23 peer-reviews [ORCID].

5. Provided mentorship to three graduate students, an MIT MSRP student, and two MIT undergraduate (UROP) students.

6. Awarded the National President's Volunteer Service Award for over 150 hours of service with Paint-a-Wish, which teaches children with disabilities to express themselves through art, crafts, and music. Leveraging my skills as a professional artist and my personal experiences with my disability, I provided children with a creative outlet for the challenges.

7. Received the Lieutenant Governor's Community Service Award for my community service as a leader in the student-led organization Cougars vs Cancer (CVC), securing a $100,000 donation for the Simmon's Center for Cancer Research (SCCR) through the INFINITI challenge award.

8. Organized the successful 2018 Rex Lee Run for a Cure, raising thousands of dollars for cancer research and attracting hundreds of participants. The event earned positive community and media attention [Press].

9. Completed a two-year humanitarian mission, serving in cities across the country such as Villarrica, Valdivia, Puerto Montt, Los Lagos, Osorno, and Lanco.

Teaching Experience

Instructor • *Biological Engineering* • 3D Scientific Rendering (20.S947)
Teaching Assistant • *Chemical Engineering* • Computational Chemistry (10.437)
Teaching Assistant • *Biological Engineering* • Principles of Molecular Bioengineering (20.420)
Teaching Assistant • *Cell Biology & Physiology* • Cell Biology (PDBIO 360)

Skills and Specializations

- Spanish (bilingual)
- Python
- Software development (GitHub)
- Molecular modeling
- Multi-scale modeling (QM/MM)
- Molecular dynamics (MD) simulations
- Quantum mechanical (QM) calculations
- Density functional theory (DFT)
- Molecular Visualization
- High-performance Computing
- Machine Learning
- NMR imaging and processing
- Cell culture and protein sample prep
- Immunohistochemistry (IHC)
- Electron and light microscopy
- Organic synthesis

Certifications

Fundamentals of Accelerated Computing with CUDA Python issued by NVIDIA
Fundamentals of Deep Learning issued by NVIDIA

Current Societal and Honors Affiliations

Society for Advancement of Chicanos/Hispanics & Native Americans in Science (SACNAS)
National Spanish Speaker Honor Society (SDP)
Hispanic Scholarship Fund (HSF)
American Chemical Society (ACS)
The Protein Society (TPS)
National Scientific Research Honor Society Sigma Xi
National Honor Society Phi Kappa Phi (PKP - Council Member)
International Honor Society Golden Key (GKHS)

Press

"Scientists use computational modeling to design "ultrastable" materials *MIT News*, **2023**.
"Computational modeling guides development of new materials" *MIT News*, **2022**.
"The Ultimate Triumph of Truth" *BYU Speeches*, **2019**.
"Part of the search: Q&A with BYU Commencement Speaker" *BYU Honors Program News*, **2019**.
"A wonderful world to share joy, show love, create connections" *BYU News*, **2019.**
"Kastner chosen as commencement speaker at BYU" *Napa Valley Register*, **2019**.
"Rex Lee Run unites those affected and impacted by cancer" *Daily Herald*, **2018**.
"Kastner receives fellowship for cancer research" *Napa Valley Register*, **2018**.
"Napa's Kastner family creates artwork for new dealership" *Napa Valley Register*, **2016**.

Highlighted Coursework

Massachusetts Institute of Technology

Biological Engineering • Protein Engineering (20.535)	Grade: A (5.0)
Biological Engineering • Analysis of Biological Networks (20.440)	Grade: A (5.0)
Computer Science • Modeling with Machine Learning: Algorithm to Apps (6.C51)	Grade: A (5.0)
Chemical Engineering • Machine Learning for Molecular Engineering (10.C51)	Grade: A (5.0)
Chemical Engineering • Computational Chemistry (10.637)	Grade: A (5.0)

Brigham Young University

Physiology • Biophysics (PDBIO 568)	Grade: A (4.0)
Physiology • Advanced Physiology (PDBIO 362)	Grade: A (4.0)
Biology • Cell Biology (BIO 360)	Grade: A (4.0)
Biology • Computational Biology (BIO 362)	Grade: A (4.0)
Chemistry • Biophysical Chemistry (CHEM 468)	Grade: A (4.0)
Chemistry • Organic Chemistry (CHEM 351 & 352)	Grade: A (4.0)
Chemistry • Biochemistry (CHEM 481)	Grade: A (4.0)
Physics • Molecular Dynamics (PDBIO 550R)	Grade: A (4.0)
Physics • Electricity and Magnetism (PHSCS 220)	Grade: A (4.0)
Physics • Newtonian and Modern Physics (PHSCS 121 & 123)	Grade: A (4.0)