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Education

Ph.D. Bioengineering	Massachusetts Institute of Technology	<i>Current</i>
B.S. Biophysics	Brigham Young University, Provo, Utah	2019
	GPA 4.0 Honors <i>Summa Cum Laude</i> , <u>Valedictorian Speech</u>	

Honors**Prestigious Awards**

Cornell Colman Inclusive Leadership Award	2021
Alfred P. Sloan Award for Exemplary Mentorship (UCEM)	2019
Lieutenant Governor's Community Service Award	2018
National President's Volunteer Service Award	2018
National Honors Society Phi Kappa Phi Outstanding Student Award	2018
Karl G. Maeser Scholarship	2018
Elva Pederson Jorgenson Award	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
Eagle Scout Award	2008

Fellowships

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

Research/Professional Experience

Pfizer Pharmaceutical Internship – Cambridge, MA Sept 2023 – Current

Advisor: Dr. Zhechun Zhang

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

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

Advisor: Dr. Heather J. Kulik

Description: PhD candidate focusing on using molecular dynamics and quantum mechanical calculations to better understand the mechanistic blueprints of reactivity in non-heme iron enzymes.

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-Myer Squibb*.**Computational and Synthetic Chemistry Researcher – Provo, UT**

Aug 2014 – Aug 2017

Advisor: Dr. Steven L. Castle**Description:** Computational chemist researching 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).**Peer-reviewed Publications**

1. 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](https://doi.org/10.1002/jcc.27242).
2. **Kastner, D.W.**; Nandy, A.; Mehmood, R.; Kulik, H.J. Mechanistic Insights into Substrate Positioning That Distinguishes Non-heme Fe(II)/ α -Ketoglutarate-Dependent Halogenases and Hydroxylases. *ACS Catal.* **2023**, 13 (4), 2489-2501. DOI: [10.1021/acscatal.2c06241](https://doi.org/10.1021/acscatal.2c06241).
3. 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](https://doi.org/10.1038/s41467-023-36299-1).
4. 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](https://doi.org/10.1021/jacsau.2c00547).
5. 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](https://doi.org/10.1021/acscatal.2c02096).
6. 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.jpcc.2c02260](https://doi.org/10.1021/acs.jpcc.2c02260).
7. 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](https://doi.org/10.1038/s41597-022-01181-0).
8. Flores, A.D.R.; **Kastner, D.W.**; Du, T.; Narayanamoorthy, M.; Shen, Y.; Cai, W.; Vennelakanti, V.; Zill, N.A.; Dell, L.B.; Zhai, R.; Kulik, H.J.; 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](https://doi.org/10.1021/jacs.1c12891).
9. 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/D1SC05992K](https://doi.org/10.1039/D1SC05992K).
10. 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](https://doi.org/10.1101/gad.348295.121).

11. 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.; Tarapsak, 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](https://doi.org/10.1016/j.ccell.2020.05.001).
12. 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 3₁₀-Helical Peptides. *J. Org. Chem.* **2020**, 3 (85), 1601-1613. DOI: [10.1021/acs.joc.9b02747](https://doi.org/10.1021/acs.joc.9b02747).
13. 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.ra119.011297](https://doi.org/10.1074/jbc.ra119.011297).
14. **Kastner, D.W.** Computational Modelling of Peptides Containing Non-Standard Amino Acids *Undergraduate Honors Thesis* **2019**. Theses. 61. ISSN: [2572-4479](https://doi.org/10.2572/4479).
15. **Kastner, D.W.** The Ultimate Triumph of Truth. *Brigham Young University Commencement*, **2019**. URL: speeches.byu.edu.
16. 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](https://doi.org/10.1016/j.ijbiomac.2018.12.218).
17. **Kastner, D.W.**; Castle, S.L. *ONIOM(DFT:MM) study of yaku'amide A and analogues*; ORCA Report. *JUR*: Provo, **2018**. URL: jur.byu.edu.
18. 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](https://doi.org/10.1021/acs.orglett.7b02455).
19. 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](https://doi.org/10.1016/j.mcp.2017.07.002).

In-Progress Publications

20. 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. *Submitted*
21. **Kastner, D.W.**; Clorice, R.; Husain, A.; Melissa, M.; Kulik, H.J. Mechanistic Insights from Dynamic Electronic Properties of Artificial Mini-Enzymes. *In preparation*.
22. **Kastner, D.W.**; Clorice, R.; Kulik, H.J. Mechanistic Insights into the Reaction of the Non-Heme Iron Enzyme DMFase. *In preparation*.
23. 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 Sprint Conference New Orleans*, **2024**. DOI: [10.1021/scimeetings.4c10442](https://doi.org/10.1021/scimeetings.4c10442).
2. **Kastner, D.W.**; Nandy, A.; Mehmoood, 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.**; Castle, S. L. ONIOM geometry optimization of bulky dehydroamino acids in β -hairpins. *IEEE Poster Session*, Provo, **2017**.

Teaching Experience

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

Skills and Specializations

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|---|--|
| • Spanish (bilingual) | • Machine Learning |
| • Python | • NMR imaging and processing |
| • Molecular Modeling | • Cell culture and protein sample prep |
| • QM/MM | • Immunohistochemistry (IHC) |
| • Molecular Dynamics | • Electron microscopy (TEM) |
| • Quantum Mechanical Calculations | • Light microscopy |
| • Molecular Visualization | • Organic synthesis |
| • High-performance Computing | • PCR |

Societal and Honors Affiliations

American Chemical Society (ACS)	2024
The Protein Society (TPS)	2023
National Scientific Research Honor Society Sigma Xi	2023
Biophysical Society (BPS)	2017
National Spanish Speaker Honor Society (SDP)	2017
National Honor Society Phi Kappa Phi (PKP - Council Member)	2016
International Honor Society Golden Key (GKHS)	2016

Relevant Coursework

Massachusetts Institute of Technology

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

Brigham Young University

<i>Physiology</i> • Biophysics (PDBIO 568)	Grade: A (4.0)
<i>Physiology</i> • Advanced Physiology (PDBIO 362)	Grade: A (4.0)
<i>Biology</i> • Cell Biology (BIO 360)	Grade: A (4.0)

<i>Biology</i> • Computational Biology (BIO 362)	Grade: A (4.0)
<i>Chemistry</i> • Biophysical Chemistry (CHEM 468)	Grade: A (4.0)
<i>Chemistry</i> • Organic Chemistry (CHEM 351 & 352)	Grade: A (4.0)
<i>Chemistry</i> • Biochemistry (CHEM 481)	Grade: A (4.0)
<i>Physics</i> • Molecular Dynamics (PDBIO 550R)	Grade: A (4.0)
<i>Physics</i> • Electricity and Magnetism (PHSCS 220)	Grade: A (4.0)
<i>Physics</i> • Newtonian and Modern Physics (PHSCS 121 & 123)	Grade: A (4.0)