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

Cornell Colman Inclusive Leadership Award	2021
National Science Foundation Graduate Research Fellowship (NSF GRFP)	2019
Alfred P. Sloan Award for Exemplary Mentorship (UCEM)	2019
Lieutenant Governor's Community Service Award	2018
National Hispanic Fund Scholarship (HSF)	2018
National President's Volunteer Service Award	2018
National Honors Society Phi Kappa Phi Outstanding Student Award	2018
National Barry Goldwater Scholarship	2017
National American Chemical Society Scholars Award (ACS)	2017
Simmons Center for Cancer Research Fellowship (SCCR)	2017

Noteworthy Awards

Vice Chancellor's Inclusive Excellence Fellowship	2020
Tolero Pharmaceuticals Fellowship	2018
Inspired Learning University Fellowship	2018
Karl G. Maeser Scholarship	2018
Elva Pederson Jorgenson Award	2018
University Undergraduate Research Award (URA)	2018
Full-Ride Merit-Based Scholarship	2017
Eagle Scout Award	2008

Research/Professional Experience

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 computational biologist. Genomic profiling of small cell, adenocarcinoma, and squamous lung cancer using genetically engineered mouse models to develop novel treatment modalities.

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

Advisor: Dr. Nico Tjandra

Description: Internship investigating fibril formation implicated in apoptosis using electron microscopy, fluorescence, and light scattering to characterize Bax-catalyzed fibrillation of an endogenous peptide.

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

Advisor: Dr. Haribabu Arthanari

Description: Internship investigating novel methods of isotopically labeling proteins by leveraging pyruvate metabolism. Involved cell culture, protein extraction, NMR, and data processing.

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

Advisor: Dr. Steven L. Castle

Description: Research assistant computationally evaluating synthetic pathways of complex peptides with non-standard residues and potent anticancer activity in collaboration with *Bristol-Myer Squibb*.

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

Advisor: Dr. Steven L. Castle

Description: Research assistant synthesizing non-standard amino acids and small peptides and predicted their structures using NMR and quantum mechanical calculations.

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

Supervisor: John E. Rappleye

Description: Full-time humanitarian volunteer serving as an entirely Spanish-speaking mission in more than 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.

2. 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 Catalysis* **2023**, 13 (4), 2489-2501. DOI: 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. *Nature Communications* **2023**, 14 (597). DOI: 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.

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 Catalysis* **2022**, 12 (15), 9281-9306. DOI: 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. *Journal Physical Chemistry B* **2022**, 126 (22), 4069-4079. DOI: 10.1021/acs.jpcb.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. *Nature Scientific Data* **2022**, 9 (74). DOI: 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, J.H.; Zhang, W. Probing the Mechanism of Isonitrile Formation by a Non-Heme Iron(II)-Dependent Oxidase/Decarboxylase. *Journal of American Chemical Society* **2022**, 144 (13), 5893-5901. DOI: 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. *Chemical Science* **2022**, 13, 1899-1905. DOI: 10.1039/D1SSC05992K.

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 & Development* **2021**, 37, 13-14. DOI: 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.; 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 Suntypes by Reprogramming Neuroendocrine Fate. *Cancer Cell* **2020**, *1* (38), 60-78. DOI: 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 3_{10}-Helical Peptides. *The Journal of Organic Chemistry* **2020**, *3* (85), 1601-1613. DOI: 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. *Journal of Biological Chemistry* **2019**, *50* (294), 19055-19065. DOI: 10.1074/jbc.ra119.0112977

14. Kastner, D.W. Computational Modelling of Peptides Containing Non-Standard Amino Acids *Undergraduate Honors Thesis* **2019**. *Theses*. 61. ISSN: 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. *International Journal of Biological Macromolecules* **2018,** 126, 229-236. DOI: 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. *Journal of Undergraduate Research (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. *Organic Letters* **2017**, *19* (19), 5190-5193. DOI: 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. *Molecular and Cellular Probes* **2017**, *36*, 21-28. DOI: 10.1016/j.mcp.2017.07.002

Conference and Poster Presentations

1. Kastner, D.W.; Nandy, A.; Mehmoood, R.; Kulik, H. 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.

2. 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**.

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

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

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

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

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

Teaching Experiences

1. Instructor • *Biological Engineering* • 3D Scientific Rendering (20.S947)

2. Teaching Assistant • *Biological Engineering* • Principles of Molecular Bioengineering (20.420)

3. Teaching Assistant • *Chemical Engineering* • Computational Chemistry (10.637)

4. Teaching Assistant • *Cell Biology & Physiology* • Cell Biology (PDBIO 360)

Skills and Specializations

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

Societal and Honors Affiliations

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

Relevant Coursework

Massachusetts Institute of Technology

Biological Engineering • Protein Engineering (20.535)	Grade: A (5.0)
Biological Engineering • Principles of Molecular Bioengineering (20.420)	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)
Mathematics • Differential and Integral Calculus (MATH 112 & 113)	Grade: A (4.0)