Kristy A. Carpenter

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Education

2020–2026*	**Ph.D.**, Biomedical Informatics, Stanford University
2016–2020	**B.S.**, Computer Science & Molecular Biology, Massachusetts Institute of Technology

Experience

Sept 2020 – present *Stanford, CA*	**Stanford University** *Graduate Researcher* Advisor: Dr. Russ Altman {machine learning, protein structure, protein-ligand binding, drug repurposing, pharmacovigilance}
June 2023 – Aug 2023 *South San Francisco, CA*	**Merck Research Laboratories** *Graduate Research Intern* Modeling & Informatics Department {machine learning, molecular dynamics, druggability}
June 2019 – Aug 2019 *Oak Ridge, TN*	**Oak Ridge National Laboratory** *Undergraduate Research Intern* Biomedical Sciences, Engineering, and Computing Group {machine learning, variational autoencoders, molecular dynamics}
Oct 2018 – May 2019 *Cambridge, MA*	**Massachusetts Institute of Technology** *Undergraduate Researcher* Advisor: Dr. Collin Stultz {machine learning, recurrent neural networks, antimicrobial peptides}
January 2018 *Charlestown, MA*	**Massachusetts General Hospital** *Undergraduate Research Intern* Advisor: Dr. Xudong Huang {machine learning, virtual screening}
June 2017 – Aug 2017 *Livermore, CA*	**Lawrence Livermore National Laboratory** *Undergraduate Research Intern* Biochemical and Biophysical Systems Group {molecular dynamics, lipids}

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*Expected.

Awards & Honors

2025	Drug Repurposing and Repositioning Insights for Treating SUDs Challenge Winner (NIH NIDA)
2023–2025	Ruth L. Kirschstein NRSA F31 Diversity (NIH NIGMS)
2021–2023	NSF Graduate Research Fellowship
2021–2022	GEM Fellowship
2020	Phi Beta Kappa
2016–2020	Koniag Education Foundation General Scholarship
2019	MakeMIT Hardware Hackathon: Top 7 Finisher
2018	MakeMIT Hardware Hackathon: Top 7 Finisher
2017–2018	AISES Northrup Grumman Academic Scholarship
2017–2018	Koniag Education Foundation Ag'wanermiut Liitut Scholarship
2016–2017	AISES Intel Scholarship
2016	HackMIT Hackathon: Best Use of Wolfram Technologies

Publications

G Google Scholar

† → Equal contribution

Journal Articles

1. Bu, F., Adam, Y., Adamiak, R. W., Antczak, M., de Aquino, B. R. H., *[...]*, **Carpenter, K. A.**, *[...]*, Westhof, E. & Miao, Z. RNA-Puzzles Round V: blind predictions of 23 RNA structures. *Nat. Methods* **22,** 399–411 (2025).

2. **Carpenter, K. A.**, Nguyen, A. T., Smith, D. A., Samori, I. A., Humphreys, K., Lembke, A., Kiang, M. V., Eichstaedt, J. C. & Altman, R. B. Which social media platforms facilitate monitoring the opioid crisis? *PLOS Digit. Health* **4,** e0000842 (2025).

3. **Carpenter, K.A.** & Altman, R. B. The Human Omnibus of Targetable Pockets. *J. Cheminf.* **17** (2025).

4. **Carpenter, K. A.** & Altman, R. B. Databases of ligand-binding pockets and protein-ligand interactions. *Comput. Struct. Biotechnol. J.* **23,** 1320–1338 (2024).

5. **Carpenter, K. A.** & Altman, R. B. Using GPT-3 to Build a Lexicon of Drugs of Abuse Synonyms for Social Media Pharmacovigilance. *Biomolecules* **13,** 387 (2023).

6. Ingólfsson, H. I., Bhatia, H., Zeppelin, T., Bennett, W. F. D., **Carpenter, K. A.**, Hsu, P.-C., Dharuman, G., Bremer, P.-T., Schiøtt, B., Lightstone, F. C. & Carpenter[*], T. S. Capturing biologically complex tissue-specific membranes at different levels of compositional complexity. *J. Phys. Chem. B* **124** (2020).

7. Chen, H. S., Jarrell, J. T., **Carpenter, K. A.**, Cohen, D. S. & Huang, X. Blockchain in Healthcare: A Patient-Centered Model. *Biomed. J. Sci. Tech. Res.* **20** (2019).

8. Cohen, D. S., **Carpenter, K. A.**, Jarrell, J. T., Huang, X. & Alzheimer's Disease Neuroimaging Initiative. Deep learning-based classification of multi-categorical Alzheimer's disease data. *Curr. Neurobiol.* **10,** 141–147 (2019).

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[*]Please note that T.S. Carpenter bears no relation to K.A. Carpenter.

9. Pang, C., Yang, H., Hu, B., Wang, S., Chen, M., Cohen, D. S., Chen, H. S., Jarrell, J. T., **Carpenter, K. A.**, Rosin, E. R. & Huang, X. Identification and Analysis of Alzheimer's Candidate Genes by an Amplitude Deviation Algorithm. *J. Alzheimers Dis. Parkinsonism* **9** (2019).

10. **Carpenter, K. A.**, Cohen, D. S., Jarrell, J. T. & Huang, X. Deep learning and virtual drug screening. *Future Med. Chem.* **10** (2018).

11. **Carpenter, K. A.** & Huang, X. Machine learning-based virtual screening and its applications to Alzheimer's drug discovery: a Review. *Curr. Pharm. Des.* **24** (2018).

12. **Carpenter, K. A.** & Huang, X. Is it a Prime Time for AI-powered Virtual Drug Screening? *EC Pharmacol. Toxicol.*, 16–17 (2017).

Peer-reviewed Conference Proceedings

13. Derry[†], A., **Carpenter**[†], **K. A.** & Altman, R. B. *Training data composition affects performance of protein structure analysis algorithms* in *Pacific Symposium on Biocomputing* (2022).

Working papers

14. Nayar, G., **Carpenter**[†], **K.A.**, Smith[†], D. A., Xiong, B. & Altman, R. B. *Exposing the Molecular Reaction Blind Spots of LLMs with PathwayQA* BioRxiv[Preprint]. 2025.

Selected Presentations

July 2025 *Stanford*, CA	"Using AI and Computational Methods for Drug Repurposing" Stanford EXPLORE Lecture Series *(invited talk)*
March 2025 *Online*	"Essential Elements for Sharing a Data Package" NIH HEAL FreshFair Webinar *(invited talk)*
June 2024 *Stanford*, CA	"Five Projects Using Social Media as an Early Warning System for the Opioid Epidemic" Stanford HAI at Five Conference *(poster)*
March 2024 *Online*	"Leveraging GPT models for Health-Related Research" Stanford TADA-BSSR T32 trainee meeting *(invited talk)*
February 2024 *Bethesda*, MD	"Which Social Media Platforms Provide the Most Informative Data for Monitoring the Opioid Crisis?" 5th Annual NIH HEAL Initiative Scientific Meeting *(poster)*
January 2023 *San Francisco*, CA	"Using the Protein Microenvironment for Computational Cryptic Pocket Prediction" UCSF QBI Full Circle Symposium *(contributed talk)*
January 2022 *Waimea*, HI	"Training data composition affects performance of protein structure analysis algorithms" Pacific Symposium on Biocomputing *(contributed talk)*

January 2022	"SiteFEATURE: Using the Protein Microenvironment for
Waimea, *HI*	Cryptic Pocket Prediction"
	Pacific Symposium on Biocomputing *(poster)*

Selected Media Coverage

2025	Stanford Department of Biomedical Data Science, Kristy Carpenter Wins the "Drug Repurposing" NIDA Challenge And May Have Solved An Even Bigger Issue With Her Research.
2019	MIT News, Computer science in service of medicine.

Teaching

Stanford University

Fall 2022	**Teaching Assistant**, Representations and Algorithms for Computational Molecular Biology *(BIOMEDIN 214 / BIOE 214 / CS 274 / GENE 214)*
Fall 2021	**Teaching Assistant**, Representations and Algorithms for Computational Molecular Biology *(BIOMEDIN 214 / BIOE 214 / CS 274 / GENE 214)*

Massachusetts Institute of Technology

Spring 2020	**Lab Assistant**, Introduction to Machine Learning *(6.036)*
Fall 2019	**Undergraduate Teaching Assistant**, Introductory Biology *(ES.7012)*
Fall 2018	**Undergraduate Teaching Assistant**, Introductory Biology *(ES.7012)*
Spring 2018	**Undergraduate Teaching Assistant**, Introductory Biology *(ES.7013)*
Fall 2017	**Undergraduate Teaching Assistant**, Introductory Biology *(ES.7012)*

Mentorship

Fall 2025	Undergraduate Researcher *(Z. Q.)*	Stanford University
Fall 2025	PhD Rotation Student *(H. C.)*	Stanford University
Fall 2024	Undergraduate Researcher *(P. G.)*	Stanford University
Spring 2024	Undergraduate Researcher *(M. L.)*	Stanford University
Spring 2023	PhD Guest Researcher *(A. S. O.)*	Stanford University

Service

Committee Member

| 2025 | Stanford Department of Biomedical Data Science Faculty Search Committee |
| 2021–2022 | Stanford Department of Biomedical Data Science Communications Committee |

Leadership

Oct 2021 – Sept 2022	**Chair**, Stanford Biomedical Informatics Student DEI Committee
Jan 2022 – Apr 2022	**Program Leader**, Stanford ADVANCE Undergraduate Institute
Jan 2021 – Apr 2021	**Program Leader**, Stanford ADVANCE Undergraduate Institute
Aug 2018 – May 2020	**Vice President**, MIT AISES Chapter

Journal Reviewer

Journal of Medical Internet Research, Journal of Structural Biology, Journal of Physical Chemistry Letters, JMIR Medical Informatics, PLOS Digital Health, Neurology: Genetics, AJPM Focus

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Last updated: December 26, 2025