Bryn Marie Reimer

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Education

University of Massachusetts Amherst — **Amherst, MA**
PhD student, Computer Science; Spaulding-Smith Fellow — *2024 – present*
Focus: Computational chemistry & biology, genomics, data science, AI/ML
Research Supervisor: Prof Anna Green, UMass Amherst

Massachusetts Institute of Technology — **Cambridge, MA**
Graduate student, Electrical Engineering and Computer Science — *2019 – 2021*
Thesis title: AI attack planning for emulated networks
Research Supervisor: Dr Una-May O'Reilly, MIT

University of Cambridge — **Cambridge, UK**
Dr Herchel Smith Fellow

Master of Philosophy in Computational Biology (Half-taught, half-research) — *2017*
Thesis title: Differential methylation in female multiple sclerosis cases
Research Supervisor: Prof Lisa Barcellos, UC-Berkeley

Master of Philosophy in Chemistry (Degree by Research) — *2016*
Thesis title: Computational studies on the mechanism of homogeneous gold catalysis
Research Supervisor: Prof Jonathan M Goodman, University of Cambridge

Williams College — **Williamstown, MA**
B.A. in Chemistry, Magna Cum Laude, Phi Beta Kappa — *2011 – 2015*

Technical Skills

Programming Languages + Related: Python (including pytorch), R and RShiny, git, LaTeX, Unix/Linux, bash, HPC cluster environments. Some experience: Java, Scala, golang, Haskell.
Broader Skills: Traditional statistical modeling (regression & classification), natural language processing, AI/ML, algorithm design and implementation, exploratory data analysis, data visualization
Computational Biology: RNAseq/DNAseq (NGS), genomics, proteomics, metabolomics
Computational Chemistry: Cheminformatics (RDKit), graphical neural nets for chemistry, molecular dynamics, virtual screening, scaffold hopping, library enumeration

Academic Awards, Fellowships, and Scholarships

Spaulding-Smith Fellow at UMass Amherst, 2025 – present	$76,000
Dr Herchel Smith Fellow at University of Cambridge, 2015–2017	$50,000
James F. Skinner Prize in Chemistry, June 2015	$500
Phi Beta Kappa Membership, June 2015	
American Physics Society / IBM Internship scholarship, Summer 2014	$6,000
CRA-W (Computing Research Association – Women) DREU scholarship, Summer 2012	$6,000

Peer-Reviewed Journal Publications

Reimer, B., ..., Hornak, V., CovCysPredictor: Predicting Selective Covalently Modifiable Cysteines Using Protein Structure and Interpretable Machine Learning. *Journal of Chemical Information and Modeling* **2025**

Gopal, R., ..., **Reimer, B.**, ..., Mootha, V.K., Effectors enabling adaptation to mitochondrial complex I loss in Hürthle cell carcinoma. *Cancer Discovery* **2023**

Shi, X.*, **Reinstadler, B.***, ... Shen, H., Combinatorial GxGxE CRISPR screening and functional analysis highlights SLC25A39 in mitochondrial GSH transport. *Nature Communications*, **2022**

Grange, RMH., ..., **Reinstadler, B.**, ..., Mootha, V.K., Zapol, W.M. Hypoxia ameliorates brain hyperoxia and NAD+ deficiency in a murine model of Leigh syndrome. *Molecular Genetics and Metabolism* **2021**

Sharma, R., **Reinstadler, B.**, ..., Mootha, V.K., Circulating markers of NADH-reductive stress correlate with mitochondrial disease severity. *The Journal of Clinical Investigation* **2021**

Wang, L.W., ..., **Reinstadler, B.**, ..., Gewurz, B.E. Epstein-Barr-virus-induced one-carbon metabolism drives B cell transformation. *Cell Metabolism* **2019**

Peer-Reviewed Workshop Papers

Nainani, J., **Reimer, B.**, Watts, C., Jensen, D., Green, AG, Mechanistic evidence that motif-gated domain recognition drives contact prediction in protein language models. *NeurIPS MechInterp Workshop* **2026**

Springer, J.*, **Reinstadler, B.***, O'Reilly, U., STRATA: Simple, Gradient-Free Attacks for Models of Code. *KDD'21 AdvML Workshop* **2021**

Selected Posters and Presentations

"Capitalizing on the AlphaFold 2 Protein Structure Modeling Breakthrough in Drug Discovery"
Reimer, B., Porter, K., Clifton, M., Hornak, V., Duca, J.
Poster presented at the Novartis Biomedical Research Retreat, **2022**

"STRATA: Building Robustness with a Simple Method for Generating Black-box Adversarial Attacks for Models of Code"
Reinstadler, B., Springer, J., O'Reilly, U.
Poster presented at NeurIPS Women in Machine Learning Workshop, **2020**

"Using clustering, meQTLs and DMR analysis to prove differences in MS cases"
Reinstadler, B., Rhead, B., Quach, H., Quach, D., Schaefer, C., Barcellos, L.F.
Poster presented at American Society of Human Genetics (ASHG) Orlando, **2017**

"P-OSRA: Polymer Optical Structure Recognition Application"
Reinstadler, B., Horn, H.
Poster presented at ACS Boston in Sci-Mix Poster Presentation, **2015**
Oral presentation given at ACS Boston in CINF division, **2015**

"Supersecondary Structure Motifs and De Novo Protein Structure Predictions"
Reinstadler, B., Van, J., Shehu, A.
Poster presented at the Grace Hopper Celebration of Women in Computing, **2012**

Research and Work Experience

Senior Expert I, Data Science || Computer-Aided Drug Discovery **Cambridge, MA**
Novartis Institutes of BioMedical Research *2021 – 2024*

- Developed CovCysPredictor for predicting covalently-modifiable cysteine residues using structural information alone
- Assessed workflows for protein-protein interaction prediction using coevolution and physics-based methods, resulting in software license recommendations and best-practices workflow development
- Co-taught in an annual lecture series on structure-based drug design using modern machine learning approaches
- Created an in-house pipeline for assessing ternary complexes with bifunctional linkers

Data Scientist **Boston, MA**
Massachusetts General Hospital *2017 – 2019*
Prof Vamsi Mootha (Harvard Medical School)

- Elucidated mitochondrial metabolism through computational genomics, metabolomics, and proteomics, working with small teams on multi-disciplinary projects, resulting in several publications
- Contributed several algorithms and pipelines that remain in use in the lab (open-source natural isotope correction; bioinformatic analysis of RNA sequencing data)
- Organized and led small symposia on statistics and hypothesis testing specifically for working biologists

Summer Intern: Software Development **Boston, MA**
Meta (since acquired by SalesForce) *Summer 2015*

- Worked with small team to develop in-house natural language processing (NLP) pipeline to tag files with content-appropriate, text-extracted concepts (Python, golang)

Summer Research: Computer vision & chem-informatics **San Jose, CA**
IBM - Almaden Research Center *Summer 2014*
Dr Hans Horn

- Successfully collaborated on image recognition software (P-OSRA) for identifying bond-line polymer structures, developing a database and database injection system using Hibernate and Maven, resulting in a functional website to field user inputs and requests to the polymer database.
- Talk on P-OSRA presented at ACS 2015

Summer Research: Structural biology **Fairfax, VA**
George Mason University *Summer 2012*
Dr Amarda Shehu

- Developed data analysis pipeline to determine whether the presence of supersecondary structural motifs in a protein could be inferred from the geometry of the secondary structure alone.
- Work resulted in a poster at the Grace Hopper Celebration for Women in Computing

Teaching & Tutoring

Teaching Assistanceships
University of Massachusetts Amherst

- INFO 390C: Intro to Computational Biology (Prof Anna Green, Fall 2025)

University of Cambridge

- Lab Demonstrator Part 1A Chemistry (Natural Sciences Tripos, 2015–2016)

Williams College

- PHIL 203: Logic and Language (Prof Keith McPartland, Spring 2015)

Lecturer (non-credit classes)
Massachusetts Institute of Technology
- English Change-Ringing: A Mathematical-Musical Team Sport
- Winter (IAP) 2021, 6 lectures

Guest Lectures
University of Massachusetts Amherst
- Substitution matrices (INFO 390C: Intro to Comp. Bio.)
- Prof Anna Green, Fall 2025, 1 lecture

Hampshire College
- Group Theory & Bell Ringing (Hampshire College Summer Studies in Math)
- Summer 2025, 1 lecture

Mount Holyoke College
- Biology, Chemistry, & ML (COMSC 235: Applications of Machine Learning)
- Prof Heather Pon-Barry, Fall 2024, 1 lecture

Novartis Biomedical Research
- From Atoms to Zebrafish: Proteins & Machine Learning (2022–2024, several lectures)

Tutoring
Williams College
- Physics tutor for the Office of Student Life (2014 – 2015)
- Private mathematics tutor (2014 – 2015)

Pedagogy training
University of Massachusetts Amherst
- COMPSCI 879: Teaching Assistants as Tomorrow's Faculty (Grade: A)

Mentorship and Service

Undergraduate Supervision
- Ivy Do, mentored 2025 at UMass. Designed and supervised a molecular machine learning project that is currently underway, with an abstract in submission at the American Chemical Society. Ivy is applying to graduate schools this fall.
- Henry Wheeler-Klainberg, mentored 2024–2025 at UMass. Henry is writing a thesis with the SAGE lab under Prof Anna Green.
- Jake Springer, mentored 2020–2021 at MIT. Designed and supervised a natural language processing project that resulted in a publication in the KDD'21 AdvML Workshop. Jake is currently a PhD student in Computer Science at CMU.

Academic & Industrial
Young Scientist Outreach Program (Novartis) *2022 – 2024*
- Collaborated with a team of volunteer organizers within Novartis to run a mentorship program for young scientists in the United States, where each young scientist was matched with a Novartis scientist mentor for the period of a year
- Coordinated and led workshops, panels, and events for the Young Scientist Outreach Program, including a 100+ person virtual event on Preparing for Graduate School
- Personally mentored several students, including monthly meetings, CV review, and mock interviewing

Bias in Coding (Novartis) *2021 – 2023*
- Together with a small team of volunteers, organized and ran workshops and events addressing the theme "Bias in Coding," writ large — how our ML models encode bias, and how our workplaces deal with interpersonal bias

Women in Machine Learning (NeurIPS workshop) *Fall 2020*

- Mentored an undergraduate student, giving technical feedback and advice through the poster process and about graduate school applications
- Volunteered to help organize conference, including coordination responsibilities overseeing a large group of volunteers

India Science Month Online (ISMO) *2020–2021*

- Mentored a PhD scholar at IISER Mohali, advising on presentation style, content, and clarity for a virtual "Talk Your Thesis" event; she went on to win second place.

Community Advocacy (Data Science)

Women in Ringing (Central Council of Church Bell Ringers) *2020–2021*

- Designed and executed data analysis and visualizations emphasizing the historical and present role of women in a traditionally male-dominated space
- Collaborated to raise awareness and introduce new initiatives supporting women in ringing, resulting in several articles, workshops, and a website full of stories: `https://www.womeninringing.info/`