Anna Gustafson Green

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University of Massachusetts
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Research Interests

Computational biology, machine learning, antibiotic resistance, bacterial genomics and evolution

Education

HARVARD UNIVERSITY ..... Cambridge, MA, USA

5/2019 **Doctor of Philosophy in Systems Biology**
Dissertation: Molecular Phenotypes from Genomic Sequences: Method Development and Biological Applications
Advisor: Prof. Debora S. Marks

UNIVERSITY OF CONNECTICUT ..... Storrs, CT, USA

5/2013 **Bachelor of Science in Molecular and Cell Biology**
Minor: Bioinformatics
Honors Thesis: Evolution of optimal growth temperature and temperature tolerance range in thermophilic bacteria
Advisor: Prof. J. Peter Gogarten

Employment History

UNIVERSITY OF MASSACHUSETTS ..... Amherst, MA, USA

9/2023 – present Assistant Professor
Director: Sequence Analysis and Genomics lab (SAGE)

HARVARD MEDICAL SCHOOL ..... Boston, MA, USA

7/2019 – 8/2023 Postdoctoral Fellow, Dept. of Biomedical Informatics

HARVARD UNIVERSITY ..... Cambridge, MA, USA

8/2013 – 5/2019 Graduate Research Assistant:
Marks Lab, Department of Systems Biology

9/2016 – 5/2018 Tutor, Bureau of Study Council:
Life Sciences 1A, Life Sciences 1B, Biological Data Analysis

UNIVERSITY OF CONNECTICUT ..... Storrs, CT, USA

9/2010 – 7/2013 Undergraduate Research Assistant:
Gogarten Lab, Molecular and Cell Biology Dept.

Honors, Awards, Fellowships

2019–20	NIH NLM Biomedical Informatics and Data Science Research Training Grant
2013–18	NSF GRFP
2017	SMBE Travel Grant
2017	Harvard Systems Biology Lynch Fellowship
2013	UConn University Scholar
2012	Barry M. Goldwater Scholarship
2011	Barry M. Goldwater Scholarship Honorable Mention

Awarded Research Grants

[G3] Machine learning to redesign antibiotics with boosted efficiency against *M. tuberculosis*

IALS Midi UMass Institute for Applied Life Sciences Midigrant
duration: January 2025 - January 2026
amount: $19,120
PIs: Anna G. Green

[G2] Forecasting antibiotic resistance using biophysics and machine learning

IRG UMass Amherst Office of the Provost Interdisciplinary Research Grants
duration: May 2024 - May 2025
amount: $50,000
PIs: Anna G. Green
Lulu Kang (Dept. of Mathematics)
Jianhan Chen (Dept. of Chemistry)

[G1] Integrating protein structure and genomic data to predict antibiotic resistance in *Mycobacterium tuberculosis*

NIH-NIAID F32 [PA-21-048] Ruth L. Kirschstein National Research Service Award (NRSA) Individual Postdoctoral Fellowship (Parent F32)
duration: July 2021 - July 2023
amount: $72,302
PIs: Anna G. Green

Research Grants Under Review

[G2] Machine-learning guided development of antibiotics that permeate the *Mtb* outer membrane

NIH R01 under review
duration: Dec 2025 - Dec 2030
amount: $ 2,978,126
MPIs: Anna G. Green and Marcos M. Pires
Co-Is: Maha R. Farhat and M. Sloan Siegrist

[G1] Improved genome-based prediction of antibiotic resistance in *Mycobacterium tuberculosis* by incorporating multi-species data

NIH R21 under review
duration: Dec 2025 - Dec 2027
amount: $ 275,000
PI: Anna G. Green

Publications

Refereed Journal Articles

* indicates shared first authorship, ** indicates senior authorship, Google Scholar

[J21] Husain Poonawala, Yu Zhang, Sravya Kuchibhotla, Anna G Green, Daniela Maria Cirillo, Federico Di Marco, Andrea Spitlaeri, Paolo Miotto, and Maha R Farhat. Transcriptomic responses to antibiotic exposure in *Mycobacterium tuberculosis*. *Antimicrobial Agents and Chemotherapy*, 68(5):e01185–23, 2024.

[J20] Anna G Green, Roger Vargas Jr, Maximillian G Marin, Luca Freschi, Jiaqi Xie, and Maha R Farhat. Analysis of genome-wide mutational dependence in naturally evolving *Mycobacterium tuberculosis* populations. *Molecular Biology and Evolution*, 40(6):msad131, 2023.

[J19] Anna G Green*, Chang Ho Yoon*, Michael L Chen, Yasha Ektefaie, Mack Fina, Luca Freschi, Matthias I Gröschel, Isaac Kohane, Andrew Beam, and Maha Farhat. A convolutional neural network highlights mutations relevant to antimicrobial resistance in *Mycobacterium tuberculosis*. *Nature communications*, 13(1):3817, 2022.

[J18] David Ding, Anna G Green, Boyuan Wang, Thuy-Lan Vo Lite, Eli N Weinstein, Debora S Marks, and Michael T Laub. Co-evolution of interacting proteins through non-contacting and non-specific mutations. *Nature ecology & evolution*, 6(5):590–603, 2022.

[J17] Anna G Green*, Hadeer Elhabashy*, Kelly P Brock, Rohan Maddamsetti, Oliver Kohlbacher, and Debora S Marks. Large-scale discovery of protein interactions at residue resolution using co-evolution calculated from genomic sequences. *Nature communications*, 12(1):1396, 2021.

[J16] Lior Artzi, Assaf Alon, Kelly P Brock, Anna G Green, Amy Tam, Fernando H Ramírez-Guadiana, Debora Marks, Andrew Kruse, and David Z Rudner. Dormant spores sense amino acids through the b subunits of their germination receptors. *Nature Communications*, 12(1):6842, 2021.

[J15] Megan Sjodt, Patricia DA Rohs, Morgan SA Gilman, Sarah C Erlandson, Sanduo Zheng, Anna G Green, Kelly P Brock, Atsushi Taguchi, Daniel Kahne, Suzanne Walker, et al. Structural coordination of polymerization and crosslinking by a seds–bpbp peptidoglycan synthase complex. *Nature microbiology*, 5(6):813–820, 2020.

[J14] John M Nicoludis*, Anna G Green*, Sanket Walujkar, Elizabeth J May, Marcos Sotomayor, Debora S Marks, and Rachelle Gaudet. Interaction specificity of clustered protocadherins inferred from sequence covariation and structural analysis. *Proceedings of the National Academy of Sciences*, 116(36):17825–17830, 2019.

[J13] Thomas A Hopf*, Anna G Green*, Benjamin Schubert*, Sophia Mersmann, Charlotta PI Schärfe, John B Ingraham, Agnes Toth-Petroczy, Kelly Brock, Adam J Riesselman, Perry Palmedo, et al. The evcouplings python framework for coevolutionary sequence analysis. *Bioinformatics*, 35(9):1582–1584, 2019.

[J12] Megan Sjodt, Kelly Brock, Genevieve Dobihal, Patricia DA Rohs, Anna G Green, Thomas A Hopf, Alexander J Meeske, Veerasak Srisuknimit, Daniel Kahne, Suzanne Walker, et al. Structure of the peptidoglycan polymerase roda resolved by evolutionary coupling analysis. *Nature*, 556(7699):118–121, 2018.

[J11] Megan Sjodt, Kelly Brock, Genevieve Dobihal, Patricia DA Rohs, Anna G Green, Thomas A Hopf, Alexander J Meeske, Veerasak Srisuknimit, Daniel Kahne, Suzanne Walker, et al. Structure and function of the seds: bpbp bacterial cell wall synthesis machinery. *Acta Crystallogr. A*, 74:a144–a144, 2018.

[J10] Rohan Maddamsetti, Philip J Hatcher, Anna G Green, Barry L Williams, Debora S Marks, and Richard E Lenski. Core genes evolve rapidly in the long-term evolution experiment with escherichia coli. *Genome Biology and Evolution*, 9(4):1072, 2017.

[J9] Adit Naor, Neta Altman-Price, Shannon M Soucy, Anna G Green, Yulia Mitiagin, Israela Turgeman-Grott, Noam Davidovich, Johann Peter Gogarten, and Uri Gophna. Impact of a homing intein on recombination frequency and organismal fitness. *Proceedings of the National Academy of Sciences*, 113(32):E4654–E4661, 2016.

[J8] John M Nicoludis, Bennett E Vogt, Anna G Green, Charlotta PI Schärfe, Debora S Marks, and Rachelle Gaudet. Antiparallel protocadherin homodimers use distinct affinity-and specificity-mediating regions in cadherin repeats 1-4. *Elife*, 5:e18449, 2016.

[J7] Yonatan H Grad, Simon R Harris, Robert D Kirkcaldy, Anna G Green, Debora S Marks, Stephen D Bentley, David Trees, and Marc Lipsitch. Genomic epidemiology of gonococcal resistance to extended-spectrum cephalosporins, macrolides, and fluoroquinolones in the united states, 2000–2013. *The Journal of infectious diseases*, 214(10):1579–1587, 2016.

[J6] Thomas A Hopf*, Charlotta PI Schärfe*, João PGLM Rodrigues*, Anna G Green, Oliver Kohlbacher, Chris Sander, Alexandre MJJ Bonvin, and Debora S Marks. Sequence co-evolution gives 3d contacts and structures of protein complexes. *elife*, 3:e03430, 2014.

[J5] Anna G Green, Kristen S Swithers, Jan F Gogarten, and Johann Peter Gogarten. Reconstruction of ancestral 16s rRNA reveals mutation bias in the evolution of optimal growth temperature in the thermotogae phylum. *Molecular biology and evolution*, 30(11):2463–2474, 2013.

[J4] Nicholas C Butzin, Pascal Lapierre, Anna G Green, Kristen S Swithers, J Peter Gogarten, and Kenneth M Noll. Reconstructed ancestral myo-inositol-3-phosphate synthases indicate that ancestors of the thermococcales and thermotoga species were more thermophilic than their descendants. *PLoS One*, 8(12):e84300, 2013.

[J3] Olga Zhaxybayeva, Kristen S Swithers, Julia Foght, Anna G Green, David Bruce, Chris Detter, Shunsheng Han, Hazuki Teshima, James Han, Tanja Woyke, et al. Genome sequence of the mesophilic thermotogales bacterium mesotoga prima mesg1. ag. 4.2 reveals the largest thermotogales genome to date. *Genome Biology and Evolution*, 4(8):812–820, 2012.

[J2] Kristen S Swithers, Gregory P Fournier, Anna G Green, J Peter Gogarten, and Pascal Lapierre. Reassessment of the lineage fusion hypothesis for the origin of double membrane bacteria. *Plos one*, 6(8):e23774, 2011.

[J1] David Williams, Gregory P Fournier, Pascal Lapierre, Kristen S Swithers, Anna G Green, Cheryl P Andam, and J Peter Gogarten. A rooted net of life. *Biology Direct*, 6:1–20, 2011.

Workshop Papers

[W1] Mahbuba Tasmin and Anna G Green**. Beyond sequence-only models: leveraging structural constraints for antibiotic resistance prediction in sparse genomic datasets. *ICLR MLGenX*, 2025.

Under Submission (not yet refereed)

[P2] Irene Lepori, Zichen Liu, Nelson Evbarunegbe, Shasha Feng, Turner P. Brown, Kishor Mane, fnu Shivangi, Mitchell Wong, Amir George, Taijie Guo, Jiajia Dong, Joel S. Freundlich**, Wonpil Im**, Anna G. Green**, Marcos M. Pires**, and M. Sloan Siegrist**. Identification of chemical features that influence mycomembrane permeation and antitubercular activity. *BiorXiv, in review at Nature Microbiology*, 2025.

[P1] Nelson Evbarunegbe, Shiyun Wa, and Anna G. Green**. Mycopermenet 2.0: Improved prediction of mycomebrane permeation using fusion noisy student self-distillation. *in review at NeurIPS*, 2025

In Preparation (not yet submitted)

[X4] Anna G. Green, Mahbuba Tasmin, Roger Vargas Jr, and Maha R. Farhat. Protein structural proximity predicts the effect of mutations on antibiotic resistance. *in preparation*, 2025.

[X3] Mahbuba Tasmin*, Saishradha Mohanty*, Sanjana G. Kulkarni, Maha R. Farhat, and Anna G. Green**. BIG-TB: A machine-learning benchmark for interpretable antibiotic resistance prediction. *in preparation*, 2025

[X2] Jatin Nainani, Bryn M Reimer, David Jensen**, and Anna G. Green**. A mechanistic explanation of contact prediction capabilities of protein language models. *in preparation*, 2025

[X1] Sanjana G. Kulkarni, Anna G. Green, Brendon C. Mann, Suchitra K. Goodwin, Samantha Malatesta, Noorjahn Rawoot, Laura White, Robin Warren, Karen R. Jacobson, and Maha R. Farhat. Convolutional neural networks quantify antibiotic resistance in *Mycobacterium tuberculosis* with diagnostic grade accuracy and learn from known and novel pathways of resistance. *in preparation*, 2025

Teaching Activities

Instructor

University of Massachusetts, Amherst

Q10 refers to 5.0-scale, student-rated "Overall rating of the instructor's teaching."
COMPSCI 690U, 692X, and INFO 390C are new courses developed by Anna Green

		2025		
COMPSCI 690U	Spring	Computational Biology and Bioinformatics	(grad)	Q10: 4.6
		2024		
COMPSCI 690U	Spring	Comp. Bio.and Bioinformatics	(grad)	Q10: 4.6
COMPSCI 692X	Fall	Seminar: ML for Biological Sequence Data	(grad)	Q10: 4.5
INFO 390C	Fall	Intro to Comp. Bio. and Bioinformatics	(ugrad)	Q10: 4.4

Guest Lecturer

University of Massachusetts, Amherst

		2024	
COMPSCI 390B	Spring	Harnessing Data Science for Societal Good	(ugrad)

Harvard Medical School

2022

MICROBI 302QC	Winter	Introduction to Infectious Disease Research	(grad)

2021

MICROBI 302QC	Winter	Introduction to Infectious Disease Research	(grad)

Teaching Assistant

Harvard University

2014

SPU 27	Fall	Science of Cooking	(ugrad)

Student Supervision

PhD Advisor

current Mahbuba Tasmin (started Spring 2024)
Saishradha Mohanty (started Summer 2024)
Nelson Iyore Evbarunegbe (started Summer 2024)
Bryn Marie Reimer (started Fall 2024)
Shiyun Wa (started Fall 2024)

Dissertation Committee Member

current	Niah Holtz	Organismic and Evolutionary Biology
current	Juhyeon Lee	Computer Science
current	Janis Rogenmoser	Microbiology, University of Zurich

PhD Student Mentoring

2023	Sanjana Kulkarni	current PhD student at Harvard Med. School
2021	Greg Raskind	current PhD student at Harvard Med. School
2021	Aashna Shah	current PhD student at Harvard Med. School

MS Student Research Mentoring

24-25	Jatin Nainani	now a software engineer at Nvidia
24-25	Shakir Sahibul	now a software engineer at Amazon
2024	Nelson Iyore Evbarunegbe	now a PhD student at UMass Amherst
2024	Saishradha Mohanty	now a PhD student at UMass Amherst
2023	Hunter Hyonghark Lee	now a software engineer at Amazon Web Services
2022	Chang Ho Yoon	now an international clinical fellow at NHS

Undergraduate Student Research Mentoring

present	Paolo Canigula (Amherst College Interdisciplinary Honors Thesis)	
present	Henry Wheeler-Klainberg (CS Honors Thesis)	
2025	Dhevin Nandyala	now an MS student in Biomedical Informatics at Yale
2025	Manya Phutela	now an MS student in CS at UMass Amherst
23-24	Shreeja Kavuri (undergraduate thesis)	now an MS student in Public Health at UNC Chapel Hill
2023	Victoria Agbeibor (HMS SIBMI intern)	now an MD student at Baylor College of Medicine
2021	Carter Nakamoto (honors thesis)	now a PhD student in Health Policy at Stanford
2018	Aashna Shah (HSB Internship)	now a PhD student at Harvard Systems Biology
2017	Benyam Alemu (HSB Internship)	now mobile applications developer for UCSD Health

Presentations

[P13] Genomics and evolution of antibiotic resistant *Mycobacterium tuberculosis*.
– Talk at UConn Molecular and Cell Biology Dept. Seminar, April 8, 2025

[P12] Forecasting antibiotic resistance using biophysics and machine learning.
– Talk at Cold Spring Harbor Probabilistic Modeling in Genomics Conference, March 7, 2025

[P11] Machine learning predicts mycomembrane permeability of diverse chemical compounds.
– Talk at Northeast Mycobacterial Cell Wall Meeting, virtual meeting, Jan 21, 2025

[P10] Machine learning to identify antibiotic resistance-causing mutations in *Mycobacterium tuberculosis* genomes.
– Talk at Biogen Machine Learning Focus Group, virtual meeting, July 9, 2024

[P9] Genomics of antibiotic resistant *Mycobacterium tuberculosis*.
– Talk at Northeast Mycobacterial Cell Wall Meeting, virtual meeting, Jan 26, 2024

[P8] Genomics and evolution of antibiotic resistance in *Mycobacterium tuberculosis*.
– Talk at UMass Amherst Microbiology Department Graduate Seminar, Amherst, MA, USA, Oct 24, 2023

[P7] Incorporating protein 3D structure with mutational patterns in *M. tuberculosis*.
– Poster at Boston Bacterial Meeting, Cambridge, MA, USA, Jun 12–13, 2023.

[P6] How to harness AI for genomic insights in drug-resistant tuberculosis.
– Invited talk at AI For Good Seminar, **link to presentation**, Feb 25, 2022.

[P5] Genome-wide detection of mutational dependence in naturally evolving *Mycobacterium tuberculosis* populations.
– Talk at Cold Spring Harbor Genome Informatics Conference, virtual due to Covid-19, Nov 3–5, 2021.

[P4] Predicting antibiotic resistance in *Mycobacterium tuberculosis* with genomic machine learning.
– Poster at Machine Learning for Healthcare, virtual due to Covid-19, Aug 7–8, 2020.

[P3] Genome-wide detection of epistasis in antibiotic resistant *Mycobacterium tuberculosis*.
– Plenary Talk at NLM BIRT conference, virtual due to Covid-19, Jun 23–24, 2020.

[P2] Genome-scale discovery of protein-protein interactions with residue-level resolution.
– Talk at Cold Spring Harbor Probabilistic Modeling in Genomics, Cold Spring Harbor, NY, USA, Nov 4–7, 2018.

[P1] Protein interactions learned from sequences.
– Poster at Society for Molecular Biology and Evolution, Yokohama, Japan, July 7–12, 2018.

Trainee Presentations

[T4] Sub-breakpoint variations in antibiotic resistance in *Mycobacterium tuberculosis* are not associated with unfavorable tuberculosis treatment outcomes.
Sanjana Kulkarni, Brendon Mann, Marie Sjölin Wijk, Samantha Malatesta, Suchitra Kulkarni Goodwin, Sarah Thomson, Anna G. Green, Noorjahn Rawoot, Robin Warren, Karen R. Jacobson, Maha Farhat
– Poster at ASM Microbe, June 19, 2025

[T3] Mycobacterial outer membrane permeation screen identifies chemical scaffolds that promote whole-cell anti-tuberculosis efficacy.
Irene Lepori, Nelson Evbarunegbe, Anna G. Green, M. Sloan Siegrist
– Poster at EFMC International Symposium on Medicinal Chemistry, Sep 1, 2024

[T2] Protein structure-informed regularized linear model outperforms esm for predicting antibiotic resistance in *Mycobacterium tuberculosis*.
Mahbuba Tasmin, Anna G. Green
– Poster at Harvard PQG AI for Genomics & Health Conference, Oct 17, 2024

[T1] Mycobacterial outer membrane permeation screen identifies chemical scaffolds that promote whole-cell anti-tuberculosis efficacy.
Nelson Evbarunegbe, Irene Lepori, M. Sloan Siegrist, Anna G. Green
– Poster at Harvard PQG AI for Genomics & Health Conference, Oct 17, 2024

Professional Service

Conference Organization

2025	
Machine Learning For Healthcare	Area Chair

Peer Reviewing

2025	
Machine Learning in Computational Biology	conference review
Advanced Science	journal peer review
Molecular Biology and Evolution	journal peer review
2024	
BMC Genome Medicine	journal peer review
BMC Infectious Diseases	journal peer review
Current Opinions in Structural Biology	journal peer review
2022	
Microbial Genomics	journal peer review
American Journal of Respiratory and Critical Care Medicine	journal peer review
2021	
PLoS Computational Biology	journal peer review
2019	
Genome Biology	journal peer review

Institutional Service

2024–2025

UMass Amherst Quad-Lab Tuberculosis Group Meeting – PI and Organizer
UMass Amherst Computational Biology Monthly Group Meeting – Co-founder and Organizer
UMass CICS Graduate Program Committee
UMass CICS Graduate Admissions Committee

2023–2024

UMass Amherst Quad-Lab Tuberculosis Group Meeting – PI and Organizer
UMass Amherst Computational Biology Monthly Group Meeting – Co-founder and Organizer
UMass CICS Graduate Program Committee
UMass CICS Graduate Admissions Committee – resulted in 200% more Spaulding-Smith Fellowships awarded