Terra Sztain, Ph.D.

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EDUCATION

Ph.D. Chemistry, University of California, San Diego	2021
B.S. Biochemistry, *cum laude*, University of California, Los Angeles	2016

PROFESSIONAL EXPERIENCE

Affiliated Faculty, Rosetta Commons	2024 – Present
Affiliated Faculty, Biophysics, University of Michigan	2024 – Present
Affiliated Faculty, Michigan Institute for Data and AI in Society, University of Michigan	2023 – Present
Affiliated Faculty, Center for Computational Medicine and Bioinformatics, University of Michigan	2023 – Present
Assistant Professor of Medicinal Chemistry, University of Michigan	2023 – Present
Postdoctoral Researcher, Freie Universität Berlin	2021 – 2023
Graduate Researcher, University California, San Diego	2016 – 2021
Undergraduate Researcher, University of California, Los Angeles	2014 – 2016
National Cancer Institute Research Fellow, City of Hope National Medical Center	2013 – 2014
Rose Hills Research Fellow, Oak Crest Institute of Science	2012 – 2013

AWARDS and HONORS

Alexander Von Humboldt Postdoctoral Fellowship	2022
D. E. Shaw Research Graduate and Postdoc Women's Fellowship	2022
Gordon Bell Special Prize for COVID-19, Finalist	2021
Outstanding Dissertation Award, University of California, San Diego	2021
Gordon Bell Special Prize for COVID-19, Winner	2020
Southern California Users of Magnets Best Poster Award	2020
Carol and George Lattimer Award for Graduate Excellence	2019
Enzymes, Coenzymes and Metabolic Pathways GRC Best Poster Award	2019
Bruno Zimm Award	2019
National Science Foundation Graduate Research Fellowship	2018 – 2021
Alfred P. Sloan Fellowship	2016 – 2021
Strategic Enhancement of Excellence through Diversity Fellowship	2016 – 2021

PUBLICATONS

1. Allemann, M. N.; Ma, S.; **Sztain, T**.; Bartholow, T. G.; Marshall, I. P. G.; McCammon, J. A.; Burkart, M.; Allen, E. E.; Bartlett, D. H.; Marietou, A. Adaptation to High Pressure; Insights from the Genome of an Evolved Escherichia Coli Strain with Increased Piezotolerance. *bioRxiv* **2024**, p 2024.09.24.613341. https://doi.org/10.1101/2024.09.24.613341

   Durumeric, A. E. P.; Köhler, J.; Elez, K.; Raich, L.; Suriana, P. A.; **Sztain, T.*** Machine Learning Driven Simulations of SARS-CoV-2 Fitness Landscape. *bioRxiv* **2024**, p 2024.09.20.614179. https://doi.org/10.1101/2024.09.20.614179. * corresponding author

2. **Sztain, T**.; Corpuz, J.; Bartholow, T.; Sanlley Hernandez, J.; Jiang, Z.; Mellor, D.; Heberlig, G.; La Clair, J.; McCammon, J. A.; Burkart, M. D. Interface Engineering of Carrier Protein–Dependent Metabolic Pathways. *ACS Chem Biol.* **2023**, *18* (9), 2014-2022. https://doi.org/10.1021/acschembio.3c00238

3. Dommer, A.; Casalino, L.; Kearns, F.; Rosenfeld, M.; Wauer, N.; Ahn, S.-H.; Russo, J.; Oliveira, S.; Morris, C.; Bogetti, A.; Trifan, A.; Brace, A.; **Sztain, T**.; Clyde, A.; Ma, H.; Chennubhotla, C.; Lee, H.; Turilli, M.; Khalid, S.; Tamayo-Mendoza, T.; Welborn, M.; Christensen, A.; Smith, D. G. A.; Qiao, Z.; Sirumalla, S. K.; O'Connor, M.; Manby, F.; Anandkumar, A.; Hardy, D.; Phillips, J.; Stern, A.; Romero, J.; Clark, D.; Dorrell, M.; Maiden, T.; Huang, L.; McCalpin, J.; Woods, C.; Gray, A.; Williams, M.; Barker, B.; Rajapaksha, H.; Pitts, R.; Gibbs, T.; Stone, J.; Zuckerman, D.; Mulholland, A.; Miller, T.; Jha, S.; Ramanathan, A.; Chong, L.; Amaro, R. #COVIDisAirborne: AI-Enabled Multiscale Computational Microscopy of Delta SARS-CoV-2 in a Respiratory Aerosol. *Int. J. High Perform. Comput. Appl.* **2023**, 37 (1), 28-44. https://doi.org/10.1177/10943420221128233

4. Bartholow, T. G.; **Sztain, T**.; Young, M. A.; Lee, D. J.; Davis, T. D.; Abagyan, R.; Burkart, M. D. Control of Unsaturation in De Novo Fatty Acid Biosynthesis by FabA. *Biochemistry* **2022**, *61* (7), 608–615. https://doi.org/10.1021/acs.biochem.2c00094

5. **Sztain, T**.; Ahn, S.-H.; Bogetti, A. T.; Casalino, L.; Goldsmith, J. A.; Seitz, E.; McCool, R. S.; Kearns, F. L.; Acosta-Reyes, F.; Maji, S.; Mashayekhi, G.; McCammon, J. A.; Ourmazd, A.; Frank, J.; McLellan, J. S.; Chong, L. T.; Amaro, R. E. A Glycan Gate Controls Opening of the SARS-CoV-2 Spike Protein. *Nat. Chem.* **2021**, *13* (10), 963–968. https://doi.org/10.1038/s41557-021-00758-3

6. Casalino, L.; Dommer, A. C.; Gaieb, Z.; Barros, E. P.; **Sztain, T**.; Ahn, S.-H.; Trifan, A.; Brace, A.; Bogetti, A. T.; Clyde, A.; Ma, H.; Lee, H.; Turilli, M.; Khalid, S.; Chong, L. T.; Simmerling, C.; Hardy, D. J.; Maia, J. D.; Phillips, J. C.; Kurth, T.; Stern, A. C.; Huang, L.; McCalpin, J. D.; Tatineni, M.; Gibbs, T.; Stone, J. E.; Jha, S.; Ramanathan, A.; Amaro, R. E. AI-Driven Multiscale Simulations Illuminate Mechanisms of SARS-CoV-2 Spike Dynamics. *Int. J. High Perform. Comput. Appl.* **2021**, *35* (5), 432–451. https://doi.org/10.1177/10943420211006452

   Sztain, T.*; Amaro, R.; McCammon, J. A. Elucidation of Cryptic and Allosteric Pockets within the SARS-CoV-2 Main Protease. *J. Chem. Inf. Model.* **2021**, *61* (7), 3495–3501. https://doi.org/10.1021/acs.jcim.1c00140.

   * corresponding author

7. **Sztain, T**.; Bartholow, T. G.; Lee, D. J.; Casalino, L.; Mitchell, A.; Young, M. A.; Wang, J.; McCammon, J. A.; Burkart, M. D. Decoding Allosteric Regulation by the Acyl Carrier Protein. *Proc. Natl. Acad. Sci. U.S.A. S* **2021**, *118* (16). https://doi.org/10.1073/pnas.2025597118

8. Bartholow, T. G.; **Sztain, T**.; Patel, A.; Lee, D. J.; Young, M. A.; Abagyan, R.; Burkart, M. D. Elucidation of Transient Protein-Protein Interactions within Carrier Protein-Dependent Biosynthesis. *Commun. Biol.* **2021**, *4* (1), 1–10. https://doi.org/10.1038/s42003-021-01838-3

9. Bartholow, T. G.; **Sztain, T**.; Young, M. A.; Davis, T. D.; Abagyan, R.; Burkart, M. D. Protein–Protein Interaction Based Substrate Control in the E. Coli Octanoic Acid Transferase, LipB. *RSC Chem. Biol.* **2021**, *2*, 1466–1473. https://doi.org/10.1039/D1CB00125F

10. **Sztain, T**.; Bartholow, T. G.; McCammon, J. A.; Burkart, M. D. Shifting the Hydrolysis Equilibrium of Substrate Loaded Acyl Carrier Proteins. *Biochemistry* **2019**, *58* (34), 3557–3560. https://doi.org/10.1021/acs.biochem.9b00612

11. **Sztain, T**.; Patel, A.; Lee, D. J.; Davis, T. D.; McCammon, J. A.; Burkart, M. D. Modifying the Thioester Linkage Affects the Structure of the Acyl Carrier Protein. *Angew. Chem., Int. Ed.* **2019**, *58* (32), 10888–10892. https://doi.org/10.1002/anie.201903815

12. Nardi, I.; Reno, T.; Yun, X.; **Sztain, T**.; Wang, J.; Dai, H.; Zheng, L.; Shen, B.; Kim, J.; Raz, D. Triptolide Inhibits Wnt Signaling in NSCLC through Upregulation of Multiple Wnt Inhibitory Factors via Epigenetic Modifications to Histone H3. *Int. J. Cancer* **2018**, *143* (10), 2470–2478. https://doi.org/10.1002/ijc.31756

13. Gunawardana, M.; Chang, S.; Jimenez, A.; Holland-Moritz, D.; Holland-Moritz, H.; La Val, T. P.; Lund, C.; Mullen, M.; Olsen, J.; **Sztain, T**. A.; Yoo, J.; Moss, J. A.; Baum, M. M. Isolation of PCR Quality Microbial Community DNA from Heavily Contaminated Environments. *J. Microbiol. Methods* **2014**, *102*, 1–7. https://doi.org/10.1016/j.mimet.2014.04.005

PRESENTATIONS

Invited Seminars

- "Dynamic design with WESTPA simulations and Rosetta" MolSSI Workshop Software Challenges for Enzyme Design, 2025
- "Combining physics and machine learning for computer-aided drug design" American Physical Society Sprint Meeting, 2025

- "Combining physics and machine learning for computer-aided design" Wayne State University Biochemistry Seminar, 2024
- "Dynamics and AI-guided Molecular Design" American Chemical Society Spring Meeting, 2024
- "Dynamics and Computer-Aided Molecular Design" Biophysics Seminar, University of Michigan 2024
- "Dynamics and AI-guided Molecular Design" Michigan Molecular Modeling Group, University of Michigan 2023
- "Alexander Von Humboldt Post-Doctoral Fellowship Application" Demystifying Post-Doctoral Research Fellowship Applications: Over Land, Over Zee, Zoom, 2023
- "Computational Drug Discovery" Berlin Science Week, Museum für Naturkunde 2022
- "Glycan Gate: Atomic-level characterization of SARS-CoV-2 spike opening" American Chemical Society Spring Meeting, 2022
- "SARS-CoV-2 glycosylated spike activation mechanism" Student Research Seminar, University of California, San Diego, 2021
- "Carrier Protein Structure and Dynamics" University of California, San Diego Chemistry and Biochemistry Department Recruitment, 2021
- "Exclusive Grants for Ethical Research" Organ-on-a-Chip Symposium, University of California, San Diego, 2017

Contributed Seminars and Posters

- (seminar) "Physics-informed machine learning for computer-aided drug design" American Chemical Society Spring Meeting, 2025
- "Nirmatrelvir Binding Mechanism Informs Resistance and Reveals Druggable Mpro Sites" Computational Chemistry Gordon Research Conference, 2024
- "Computer-Aided Biosynthetic Pathway Engineering" Biophysical Society Annual Meeting, 2024
- "Machine learning-driven simulations of SARS-CoV-2 receptor binding domain evolution" Computational Chemistry Gordon Research Conference, 2022
- (seminar) "Weighted Ensemble Simulations of SARS-CoV-2 Glycosylated Spike Opening" Computer Simulation and Theory of Macromolecules, 2022
- (seminar) "SARS-CoV-2 glycosylated spike activation mechanism – simulations of the full unbiased pathway" Biophysical Society Annual Meeting, *Featured*, 2021
- "Decoding the Allosteric Nature of Acyl Carrier Proteins" Southern California Users of Magnets, 2020, ***Best Poster Award***
- "Effect of Cargo Identity on Acyl Carrier Protein Structure" Biophysical Society Annual Meeting, 2020
- "Computational and Spectroscopic Investigation of Communication Mechanisms used by Acyl Carrier Proteins" Enzymes, Coenzymes and Metabolic Pathways GRC, 2019, ***Best Poster Award***
- "Computational and Spectroscopic Investigation of Communication Mechanisms used by Acyl Carrier Proteins" Biophysical Society Annual Meeting, 2019
- "Epigenetics in doxorubicin and docetaxel-resistant triple negative breast cancer" American Association for Cancer Research Annual Meeting, 2016
- "Triptolide Restores WIF1 Expression by DNA Demethylation in Non-Small Cell Lung Cancer Cells" Eugene and Ruth Roberts Summer Student Academy, City of Hope 2014
- (seminar) "Metagenomic Analysis of Asphalt" Rose Hills Fellows Seminar Day, Huntington Library, 2014

TEACHING

University of Michigan

Course Coordinator, Machine Learning for Drug Discovery	2025
Instructor, Drug Discovery	2025
Instructor, Biophysical Chemistry 1 (Methods and Techniques)	2024

University of California San Diego

Teaching Assistant, Organic Chemistry Laboratory	2017
Teaching Assistant, Biochemical Structure and Function	2016

MENTORING

Postdoctoral Researchers
Mortaza Derakhshani Molayousefi (2024)
PhD Students

Luxuan Wang (2025), Daniel Santos-Perez (2024) Yao Fu (2024), Ileanexis Madera Cueves (2024), Marissa Dolorfino (2024)
PharmD Students
Jay Smith (2024)
Undergraduate Students
Zoha Rizvi (2025), Malik Alabbas (2024), Schuyler Byrn (2024)

Alumni
Nazifa Kadir (2024 – 2025)
Sean McCarty (2023 – 2024; now Senior Scientist, EyeCRO)
Jason Lin (2023 – 2024; now PhD, University of North Carolina at Chapel Hill)

SERVICE

Peer Review – Biochemistry; Frontiers in Microbiology; Journal of Chemical Information and Modeling; Journal of Molecular Graphics and Modeling; Proteins: Structure, Function, and Bioinformatics
Professional Societies – American Chemical Society, American Physical Society, Biophysical Society, Rosetta Commons
University of Michigan
Co-chair, Faculty Search Committee, 2025
Member, Faculty Development Committee, 2025
Member, PhD Admissions Committee (Medicinal Chemistry), 2024, 2025
Member, PhD Admissions Committee (Biophysics), 2025
Co-organizer, Michigan Molecular Modeling Supergroup, 2023 – Present