

# Terra Sztain, Ph.D.

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## EDUCATION

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<b>Ph.D. Chemistry</b> University of California, San Diego Thesis: Biophysical investigation of acyl-carrier and SARS-CoV-2 protein communication mechanisms	2021
<b>B.S. Biochemistry, <i>cum laude</i></b> University of California, Los Angeles	2016

## RESEARCH EXPERIENCE

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<b>Postdoctoral Researcher</b> Freie Universität Berlin Advisor: Frank Noé, Ph.D. <ul style="list-style-type: none"><li>Using AI to predict the effect of mutations on protein structure and function.</li></ul>	2021 – Present
<b>Graduate Researcher</b> University of California, San Diego Advisors: Michael Burkart, Ph.D., J. Andrew McCammon, Ph.D. <ul style="list-style-type: none"><li>Studied protein communication mechanisms - structural modifications, protein-protein interactions, and conformational changes using nuclear magnetic resonance spectroscopy and molecular dynamics simulations.</li></ul>	2016 – 2021
<b>Undergraduate Researcher</b> University of California, Los Angeles Advisor: Helena Chang, M.D., Ph.D. <ul style="list-style-type: none"><li>Designed budget and protocol for independent project studying histone epigenetics of genes involved in drug resistance and stem-cell-likeness in triple negative breast cancer using chromatin immunoprecipitation-qPCR.</li></ul>	2014 – 2016
<b>National Cancer Institute Research Fellow</b> City of Hope National Medical Center Advisor: Dan Raz, M.D. <ul style="list-style-type: none"><li>Elucidated Wnt Inhibitory Factor 1 gene promoter demethylation as an anti-tumor mechanism of the natural product triptolide.</li></ul>	2013 – 2014
<b>Rose Hills Research Fellow</b> Oak Crest Institute of Science Advisor: Mark Baum, Ph.D. <ul style="list-style-type: none"><li>Optimized protocol for DNA extraction and analyzed functional genes present in a microbial community of extremophiles from natural tar pits.</li></ul>	2012 – 2013

## FELLOWSHIPS

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National Science Foundation Graduate Research Fellowship	2018 – 2021
Alfred P. Sloan Fellowship	2016 – 2021
Strategic Enhancement of Excellence through Diversity Fellowship	2016 – 2021

## HONORS and AWARDS

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D. E. Shaw Research Graduate and Postdoc Women's Fellowship	2022
Outstanding Dissertation Award, University of California, San Diego	2021
Carol and George Lattimer Award for Graduate Excellence	2019
Bruno Zimm Award	2019
College Sponsorship Program, United Friends of the Children	2014 – 2016
Dean's Honors, 4 Quarters, University of California, Los Angeles	2014 – 2016
Twanna and John Rogers Award	2015
Niel McDowell Trust Scholarship	2015
Sam B. Jameson Scholarship	2014
Pritzker Family Foster Youth Scholarship	2014
Continuing Education Scholarship, Los Angeles County	2012 – 2014
Dean's Honors, 4 Semesters, Pasadena City College	2011 – 2014
Bernard Osher Scholarship	2013
Ebell Scholarship	2012
General Scholarship, Pasadena City College	2012

## TEACHING and MENTORSHIP

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### Teaching Assistant

Organic Chemistry Laboratory	2017
Biochemical Structure and Function	2016

### Mentor/ Supervisor

#### Undergraduate Researchers

- Andrew Mitchell - Currently pursuing **Chemistry PhD at Stanford**. 2019 – 2021

#### High School Researchers

- Kyra Wu -**1st place** in the Senior Division, Biochemistry Greater San Diego Science and Engineering Fair (GSDSEF), and nominated to go on to the California Science and Engineering Fair (CSEF). 2019 – 2021

## PUBLICATIONS

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1. 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.* **2022**, (in press). Preprint: <https://doi.org/10.1101/2021.11.12.468428>
2. 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>
3. **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>
4. 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>

5. **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>
6. **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>
7. 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>
8. 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>
9. **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>
10. **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>
11. 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>
12. 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>

## CONFERENCE PROCEEDINGS

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### Presentations

1. “Weighted Ensemble Simulations of SARS-CoV-2 Glycosylated Spike Opening” Computer Simulation and Theory of Macromolecules, April 8<sup>th</sup>, 2022
2. “Glycan Gate: Atomic-level characterization of SARS-CoV-2 spike opening” American Chemical Society Spring Meeting, March 20<sup>th</sup>, 2022
3. “SARS-CoV-2 glycosylated spike activation mechanism” Student Research Seminar, University of California, San Diego March 3<sup>rd</sup>, 2021
4. “SARS-CoV-2 glycosylated spike activation mechanism – simulations of the full unbiased pathway” Biophysical Society Annual Meeting 2021 February 25<sup>th</sup>, 2021 **Featured**
5. “Carrier Protein Structure and Dynamics” University of California, San Diego Chemistry and Biochemistry Department Recruitment, February 12<sup>th</sup> 2021
6. “Exclusive Grants for Ethical Research” Organ-on-a-Chip: a more ethical, economical, and effective model Symposium, University of California, San Diego, CA, May 19<sup>th</sup>, 2017
7. “Metagenomic Analysis of Asphalt” Rose Hills Fellows Seminar Day, Pasadena, CA, July 12<sup>th</sup>, 2014

### Posters

8. “Machine learning-driven simulations of SARS-CoV-2 receptor binding domain evolution” Computational Chemistry Gordon Research Conference July 2022
9. “Decoding the Allosteric Nature of Acyl Carrier Proteins” Southern California Users of Magnets, August 2020, **Best Poster Award**
10. “Effect of Cargo Identity on Acyl Carrier Protein Structure” Biophysical Society Annual Meeting, February 2020

11. “Computational and Spectroscopic Investigation of Communication Mechanisms used by Acyl Carrier Proteins” Enzymes, Coenzymes and Metabolic Pathways GRC, July 2019, ***Best Poster Award***
12. “Computational and Spectroscopic Investigation of Communication Mechanisms used by Acyl Carrier Proteins” Biophysical Society Annual Meeting, March 2019
13. “Epigenetics in doxorubicin and docetaxel-resistant triple negative breast cancer” American Association for Cancer Research Annual Meeting, New Orleans, LA, April 2016
14. “Triptolide Restores WIF1 Expression by DNA Demethylation in Non-Small Cell Lung Cancer Cells” Eugene and Ruth Roberts Summer Student Academy, Duarte, CA, July 2014

## SERVICE and LEADERSHIP

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### Peer Review

Biochemistry  
 Frontiers in Microbiology  
 Journal of Chemical Information and Modeling  
 Journal of Molecular Graphics and Modeling  
 Proteins: Structure, Function, and Bioinformatics

### Service Positions at UCSD

Organ-on-a-Chip Symposium at UCSD, Founder, Advisor	2016 – Present
Diversity Advisory Council to Graduate Student Association, Member	2018 – 2021
Hope Scholars, Member	2018 – 2021
Triton Recovery Group, President	2017 – 2020
Student-led Seminar Committee, Member	2017 – 2018
Graduate Student Association, Chemistry Representative	2017 – 2018

### Service Positions at UCLA

Gymnastics Club Team, Vice President	2015 – 2016
Bruins for Recovery, Member	2014 – 2016
Bruin Guardian Scholars, Member	2014 – 2016