

# Terra Sztain, Ph.D.

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## EDUCATION

**Ph.D. Chemistry** 2021  
University of California, San Diego

**B.S. Biochemistry, *cum laude*** 2016  
University of California, Los Angeles

## RESEARCH EXPERIENCE

**Postdoctoral Researcher** 2021 – Present  
Freie Universität Berlin  
Advisor: Frank Noé, Ph.D.

- Developing machine learning algorithms to engineer proteins

**Graduate Researcher** 2016 – 2021  
University of California, San Diego  
Advisors: Michael Burkart, Ph.D., J. Andrew McCammon, Ph.D.

- Studied protein structure, and protein-protein interactions through molecular dynamics simulations and nuclear magnetic resonance spectroscopy.
- Re-engineered acyl carrier protein dependent pathways for biosynthetic products.
- Performed enhanced sampling simulations of SARS-CoV-2 proteins

**Undergraduate Researcher** 2014 – 2016  
University of California, Los Angeles  
Advisor: Helena Chang, M.D., Ph.D.

- Designed budget and protocol for independent project.
- Studied histone epigenetics of promoter regions of genes involved in drug resistance and stem-cell-likeness in triple negative breast cancer upon chemotherapeutic treatment.
- Used chromatin immunoprecipitation-qPCR to compare changes in nucleosome density and H3K9 acetylation and methylation patterns.

**National Cancer Institute Research Fellow** 2013 – 2014  
City of Hope National Medical Center  
Advisor: Dan Raz, M.D.

- Elucidated Wnt Inhibitory Factor 1 gene promoter demethylation as an anti-tumor mechanism of the natural product triptolide.
- Analyzed methylation patterns through bisulfite conversion, cloning, and sequencing.

**Rose Hills Research Fellow** 2012 – 2013  
Oak Crest Institute of Science  
Advisor: Mark Baum, Ph.D.

- Optimized protocol for DNA extraction, and analyzed the functional genes present in a microbial community of extremophiles from natural tar pits.

## FELLOWSHIPS

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

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

## TEACHING and MENTORSHIP

### Teaching Assistant

Organic Chemistry Laboratory	2017
<ul style="list-style-type: none"><li>Supervise students performing laboratory experiments, wrote and graded quizzes, graded exams, and lab reports.</li></ul>	
Biochemical Structure and Function	2016
<ul style="list-style-type: none"><li>Facilitated discussion on lecture topics, group problem solving, and graded problem sets.</li></ul>	

### Mentor/ Supervisor

#### Undergraduate Researchers

- Andrew Mitchell - designed and supervised project of high-throughput virtual screening combined with ensemble docking for protein-protein inhibitors for *Mycobacterium tuberculosis* proteins, publication in preparation. Currently pursuing Chemistry PhD at Stanford. 2019 – Present
- Jianing Wang - guided through computation procedures including molecular dynamics simulations of proteins with covalent ligands. 2018 – 2019

#### High School Researchers

- Kyra Wu - guiding computational high-throughput virtual screen project, and experimental validation. **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 – Present
- BioChemCoRe - lectured and led tutorial on hydrogen bond analysis from molecular dynamics simulations. 2018

## PUBLICATIONS

- 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 (In Press 2021)*.
- Sztain, T.**, Ahn, S-H., Bogetti, A.T., Casalino, L., Goldsmith, J.A., McCool, R.S., Kearns, F.L., McCammon, J.A., McLellan, J.S., Chong, L.T., Amaro R.E., A glycan gate controls opening of the SARS-CoV-2 spike protein. *Nature Chemistry* (2021)
- 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. Bio.* (2021). doi:[10.1039/D1CB00125F](https://doi.org/10.1039/D1CB00125F).

4. **Sztain, T.\***, Amaro, R., McCammon, J.A., Elucidation of cryptic and allosteric pockets within the SARS-CoV-2 protease. *J. Chem. Inf. Model.* **61**, 3495–3501 (2021). **Cover Art** \*corresponding author
5. **Sztain, T.**, Bartholow, T.G., Lee, D.J., Casalino, L., Mitchell, A., Young, M., Wang, J., McCammon J.A., Burkart, M.D. Decoding the allosteric nature of acyl carrier proteins. *PNAS.* **118**, (2021).
6. Casalino, L.; Dommer, A.; Gaieb, Z.; Barros, E. P.; **Sztain, T.**; Ahn, S.-H.; Trifan, A.; Brace, A.; Bogetti, A.; Ma, H.; Lee, H.; Turilli, M.; Khalid, S.; Chong, L.; Simmerling, C.; Hardy, D. J.; Maia, J. D. C.; Phillips, J. C.; Kurth, T.; Stern, A.; Huang, L.; McCalpin, J.; 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). **Gordon Bell Prize**
7. Bartholow, T.G., **Sztain, T.**, Patel, A., Lee, D.J., Young, A.M., Abagayan, R., Burkart, M.D. Elucidation of transient protein-protein interactions within carrier protein-dependent biosynthesis *Commun. Biol.* **4**, 1–10 (2021).
8. **Sztain, T.**, Bartholow, T.G., McCammon, J.A., Burkart, M. D. Shifting the Hydrolysis Equilibrium of Substrate Loaded Acyl Carrier Proteins. *Biochemistry* **58**, 3557–3560 (2019). **Cover Art**
9. **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. *Angewandte Chemie International Edition* **58**, 10888–10892 (2019).
10. 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* **143**, 2470–2478 (2018).
11. Gunawardana M., Chang S., Jimenez A., Holland-Moritz D., Holland-Moritz H., La Val T.P., Lund C., Mullen M., Olsen J., **Sztain T.**, Yoo J., Moss J.A., Baum M.M. Isolation of PCR quality microbial community DNA from heavily contaminated environments. *J. Microbiol. Methods* **102**, 1–7 (2014).

## CONFERENCE PROCEEDINGS

### Presentations

#### Invited:

“SARS-CoV-2 glycosylated spike activation mechanism” Student Research Seminar, University of California, San Diego March 3<sup>rd</sup>, 2021

“Carrier Protein Structure and Dynamics” University of California, San Diego Chemistry and Biochemistry Department Recruitment, February 12<sup>th</sup> 2021

#### Contributed:

“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**

“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

“Metagenomic Analysis of Asphalt” Rose Hills Fellows Seminar Day, Pasadena, CA, July 12<sup>th</sup>, 2014

### Posters

“Decoding the Allosteric Nature of Acyl Carrier Proteins” Southern California Users of Magnets, August 29<sup>th</sup>, 2020, **Best Poster Award**

“Effect of Cargo Identity on Acyl Carrier Protein Structure” Biophysical Society Annual Meeting, February 19<sup>th</sup>, 2020

“Computational and Spectroscopic Investigation of Communication Mechanisms used by Acyl Carrier Proteins”  
 Enzymes, Coenzymes and Metabolic Pathways GRC, July 25<sup>th</sup>, 2019, **Best Poster Award**  
 “Computational and Spectroscopic Investigation of Communication Mechanisms used by Acyl Carrier Proteins”  
 Biophysical Society Annual Meeting, March 4<sup>th</sup>, 2019  
 “Epigenetics in doxorubicin and docetaxel-resistant triple negative breast cancer” American Association for Cancer  
 Research Annual Meeting, New Orleans, LA, April 20<sup>th</sup>, 2016  
 “Triptolide Restores WIF1 Expression by DNA Demethylation in Non-Small Cell Lung Cancer Cells” Eugene and  
 Ruth Roberts Summer Student Academy, Duarte, CA, July 30<sup>th</sup>, 2014

## SERVICE and LEADERSHIP

### Reviewer

Journal of Chemical Information and Modeling  
 Biochemistry  
 Journal of Molecular Graphics and Modeling

### Symposium Organizer

Organ-on-a-Chip Symposium at UCSD 2016 – Present

### Service Positions at UCSD

Diversity Advisory Council to Graduate Student Association, Member	2018 – 2021
Hope Scholars, Member	2018 – 2021
Triton Recovery Group, President	2017 – 2021
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

## REFERENCES

Available upon request.