

## Terra Sztain

9500 Gilman Drive • La Jolla, CA 92093, USA • 424-365-2108 • [tsztainp@ucsd.edu](mailto:tsztainp@ucsd.edu)

### EDUCATION

**Ph.D. Biochemistry and Biophysics** 2016 – 2021  
University of California, San Diego

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

### RESEARCH EXPERIENCE

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

- Studying protein structure, and protein-protein interactions through molecular dynamics simulations and nuclear magnetic resonance spectroscopy.
- Elucidating the communication mechanisms between acyl carrier proteins and their partners to re-engineer biosynthetic products.
- 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 analysis.

**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         | 2018-2020      |
| Alfred P. Sloan Fellowship                                       | 2016 – Present |
| Strategic Enhancement of Excellence through Diversity Fellowship | 2016 – Present |

## HONORS and AWARDS

|  |             |
|--|-------------|
| 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

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|--|------|
| 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   |                |
| <ul style="list-style-type: none"> <li>Andrew Mitchell - designed and supervised project of high-throughput virtual screening combined with ensemble docking for protein-protein inhibitors for <i>Mycobacterium tuberculosis</i> proteins, publication in preparation. Currently pursuing Chemistry PhD at Stanford.</li> </ul>                    | 2019 – Present |
| <ul style="list-style-type: none"> <li>Jianing Wang - guided through computation procedures including molecular dynamics simulations of proteins with covalent ligands.</li> </ul>  | 2018 – 2019    |
| High School Researchers   |                |
| <ul style="list-style-type: none"> <li>Kyra Wu - guiding computational high-throughput virtual screen project, and experimental validation. <b>1st place</b> 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).</li> </ul> | 2019 – Present |
| <ul style="list-style-type: none"> <li>BioChemCoRe - lectured and led tutorial on hydrogen bond analysis from molecular dynamics simulations.</li> </ul>  | 2018           |

## PUBLICATIONS

1. 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)*.
2. 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. (In Review 2021)*.
3. **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 (In Review 2021)*
4. **Sztain, T.**, Amaro, R., McCammon, J.A., Elucidation of cryptic and allosteric pockets within the SARS-CoV-2 protease. *JCIM (In Press 2021)*.
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., Abagyan, 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

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

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

## UNIVERSITY LEADERSHIP

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|--|----------------|
| Diversity Advisory Council to Graduate Student Association, Member | 2018 – Present |
| Hope Scholars, Member  | 2018 – Present |
| Triton Recovery Group, President                                   | 2017 – Present |
| Organ-on-a-Chip Symposium at UCSD Committee, Founder               | 2016 – Present |
| Student-led Seminar Committee, Member                              | 2017 – 2018    |
| Graduate Student Association, Chemistry Representative             | 2017 – 2018    |
| Gymnastics Club Team, Vice President                               | 2015 – 2016    |
| Bruins for Recovery, Member  | 2014 – 2016    |
| Bruin Guardian Scholars, Member                                    | 2014 – 2016    |

## REFERENCES

### Michael Burkart, Ph.D.

Professor and Teddy Traylor Faculty Scholar  
 Department of Chemistry and Biochemistry  
 University of California, San Diego  
 Pacific Hall rm 6100A  
 9500 Gilman Dr.  
 La Jolla, CA 92093-0358  
 858-534-5673  
[mburkart@ucsd.edu](mailto:mburkart@ucsd.edu)

### J. Andrew McCammon, Ph.D.

Joseph E. Mayer Professor of Theoretical Chemistry  
 Distinguished Professor of Pharmacology  
 University of California at San Diego

Urey Hall 4246  
858-534-2905  
[jmccammon@ucsd.edu](mailto:jmccammon@ucsd.edu)

**Rommie E. Amaro, Ph.D.**

Distinguished Professorship in Theoretical and Computational Chemistry  
Department of Chemistry and Biochemistry  
University of California, San Diego  
3234 Urey Hall, MC-0340  
La Jolla, CA 92093-0340  
858-534-9629  
[ramaro@ucsd.edu](mailto:ramaro@ucsd.edu)