# Christian Seitz

## Education

**University of California, San Diego (UCSD)**, La Jolla, CA, USA — Expected December 2022
PhD Candidate in Biochemistry & Biophysics, specialization in Multiscale Biology
**Elon University**, Elon, NC, USA — May 2016
Bachelor of Science in Chemistry, *Cum Laude*

## Research Interests

At the forefront of life, technology, and many areas of research, computational methods are consistently increasing in applicability and power. I am interested in both exploiting this expanding power to answer problems in global diseases such as influenza, SARS-CoV-2, tuberculosis, and HIV. A key focus of my research is linking together different scales and disciplines in science. Protein dynamics can be seen through molecular dynamics, while accessible timescales can be extended further through techniques such as Markov state models, Gaussian accelerated molecular dynamics and elastic network models. My PhD uses a wide variety of techniques to investigate global diseases, from gaining a better understanding of the proteins involved all the way through to drug development.

## UCSD PhD thesis work, member of the McCammon and Amaro labs

**Synopsis:** Computational approaches for the study of global diseases

Half of my thesis work has focused on how glycans affect the influenza glycoproteins hemagglutinin (HA) and neuraminidase (NA) using molecular dynamics, Markov state models and Brownian dynamics. I have published a study on how glycans affect drug binding to NA, submitted a study on how glycans affect the conformational accessibility of HA and NA, and are about to submit a third study on how glycans modulate binding pockets in HA. The other half of my thesis work is a potpourri of biophysics topics and techniques. I have published a study in the dynamics of the proto-nucleus wall in bacteria, and am preparing manuscripts on potential inhibitors for SARS-CoV-2, e. coli, and tuberculosis, and submitted a manuscript on probes for Alzheimer's disease.

## Publications and submitted manuscripts

**Seitz, C.***, Kochanek, S.*, Durrant, J., Casalino, L., Amaro, R.E. Cell-scale Markov state models characterize the structural and dynamical basis of Group 1 influenza fusion inhibition. *Submission to Nature Chemistry ~8/30/2022*

Casalino, L., **Seitz, C.**, Lederhofer, J., Tsybovsky, Y.; Wilson, I.A.; Kanekiyo, M., Amaro, R.E. Breathing and tilting: the flexibility of influenza glycoproteins reveals their vulnerabilities. *Submitted to Science*

Shivkumar, A.*, Berg, K.*, Sibucao, K.*, Leriche, G., Espinoza, C., Dozier, L., Patrick, G., Gaieb, Z., **Seitz, C.**, Amaro, R.E., Park, H.-H., Hoe, H.-S., Wozniak, J., Gonzalez, D., Yang, J. Nootropic Benzothiazoles Promote Dendritic Spine Formation by Targeting Fascin-1. *Submitted to Nature Chemical Biology*

Laughlin, T.G.*, Deep, A.*, Prichard, A.M., **Seitz, C.**, Gu, Y., Enustun, E., Suslov, S., Khanna, K., Birkholz, E.A., Armbruster, E., McCammon, J.A., Amaro, R.E., Pogliano, J., Corbett, K.D., Villa, E. Architecture and self-assembly of the jumbo bacteriophage nuclear shell. *Nature,* **2022**, *608*. **DOI:** 10.1038/s41586-022-05013-4

Ahn, S.-H.*, **Seitz, C***, Cruzeiro, V.D.W., McCammon, J.A., Götz, A.W. Data for molecular dynamics simulations of Escherichia coli cytochrome bd oxidase with the Amber force field. *Data in Brief,* **2021**, *38*. **DOI:** 10.1016/j.dib.2021.107401

**Seitz, C**., Casalino, L., Konecny, R., Huber, G., Amaro, R.E., McCammon, J.A. Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase. *Biophys. J.*, **2020**, *119* (11), pp 2275-2289. **DOI:** 10.1016/j.bpj.2020.10.024

**Seitz, C.G**., Zhang, H., Mo, Y., Karty, J.M. Why Do Enolate Anions Favor O-Alkylation in the Gas Phase? The Roles of Resonance and Inductive Effects in the Gas-Phase $S_N2$ Reaction between the Acetaldehyde Enolate Anion and Methyl Fluoride. *J. Org. Chem.*, **2016**, *81* (9), pp 3711-3719. **DOI:** 10.1021/acs.joc.6b00351

## Other Research Experience

**California Institute of Technology (Caltech), Pasadena, CA** June 2015 – June 2017
*Undergraduate summer researcher through the Amgen Scholars Program, work continued afterwards*
*Mentor: Prof. William A. Goddard III*

- Computationally predicted the 3D structures of three olfactory receptors
- Incorporated previously-completed experimental testing of agonists/non-agonists
- Attended meetings relating to professional development, communication and careers in science
- Attended a mid-summer symposium with the nine other US Amgen sites, which involved exploring careers in industry, presenting a chalk talk my research, networking, and an industry site visit
- Orally presented research three times and presented a poster two times

**Elon University, Elon, NC** Feb 2014 – May 2016
*Undergraduate researcher through Elon's prestigious Lumen Prize program*
*Mentor: Prof. Joel Karty*

- Analyzed the contributions to the reactivity of the enolate anion using quantum mechanical simulations
- Published a first author paper in the Journal of Organic Chemistry
- Orally presented research five times and presented a poster five times

**Rheinisch-Westfälische Technische Hochschule (RWTH) Aachen University, Germany** May 2014 – July 2014
*Undergraduate Research Opportunities Program (UROP) International Participant*
*Mentor: Prof. Alexander Böker*

- Helped synthesize a non-toxic hydrogel drug delivery system for cancer using a Schlenk line, lyophilizer, centrifuge, sonicator, rotovap, plasma machine and microfluidics setup
- Helped characterize it through IR, NMR, UV-vis, SEC and SEM
- Designed, performed, and analyzed an experiment to test how acidity influences hydrogel formation
- Orally presented research five times and presented a poster five times

## Professional Outreach, Mentoring and Leadership

**Chemistry Peer Advisory League (ChemPALs), UCSD, La Jolla, CA** October 2016 – September 2021
*Co-President, mentor*

- Mentorship organization for chemistry and biochemistry undergraduates
- Organize workshops, socials, mixers to promote interactions between graduate and undergraduate students

**EXPAND computational sciences mentorship program, UCSD, La Jolla, CA** November 2020 – June 2021
*Founding member and mentor*

- Selected from a campus-wide interview process to be one of three program mentors
- Mentored undergraduates with no computational experience through self-designed project

**Equity-Minded Leadership certificate program, UCSD, La Jolla, CA** April 2021 – June 2021
*Participant and certificate recipient*

- Studied how power, privilege, oppression, identity and equity affect leadership
- Developed an understanding of the dimensions of diversity and social justice

**iLead Program, UCSD, La Jolla, CA** March 2021 – June 2021
**LEAD (Leadership Education and Development) Program, Elon University, Elon, NC** January 2013 – May 2016
*Participant*

- Developed leadership skills while focusing on becoming a leader in the community
- Attended workshops and learned different leadership styles and how to implement them

**ComSciCom-SanDiego. Two day event, UCSD, La Jolla, CA** September 2020

**Communicating Your Research Workshop. Four day event, UCSD, La Jolla, CA** July 2017
*Participant*

- Did experiential practice in transmitting and performing your results to an audience
- Learned how metaphors, similes, and other language can be used to effectively communicate

**Chemistry Graduate Student Council (CGSC), UCSD, La Jolla, CA** May 2016 – April 2019
*Founding member and class-year representative, elected twice*

- Founded a seminar series allowing graduate students to give formal oral presentations
- Met with the administration to improve the new graduate student orientation

**Leadership & Teamwork certificate program, UCSD, La Jolla, CA** September 2017 – March 2018
*Participant and certificate recipient*

- Team-based experiential leadership program with lecture and practicum components
- Improved self-awareness of leadership styles and how they influence team development

## Awards and Recognitions

**Successful fellowship and research applications**

- XSEDE research allocation (co-PI through NSF GRFP) July 2020, April 2021
- XSEDE education allocation (co-PI through NSF GRFP) November 2020
- NSF Graduate Research Fellowship Program recipient April 2018
- NDSEG finalist April 2018
- Interfaces Graduate Program (UCSD) – only new department candidate awarded funding June 2017
- Fulbright Alternate/DAAD finalist for a one-year research stay in Germany March 2016
- Amgen Scholar (Caltech) – 7% nationally awarded funding for a 10 week research internship March 2015
- Glen Raven Scholarship (Elon) – given annually to 6 students October 2014/2015
- Fall 2014 Goldwater Scholarship Nominee October 2014
- Lumen Prize (Elon) – given annually to 15 rising juniors, Elon's highest undergraduate prize March 2014
- UROP International (RWTH Aachen) – funding for a 10-week research internship February 2014

**Honor Awards**

- Molecular Sciences Software Institute Summer School (competitive application) June 2017
- Fall 2016 TA Excellence Award (UCSD), recognizing excellence in teaching March 2017
- Pi Delta Phi, National French Honor Society (top 35% of French class) February 2015
- Phi Eta Sigma, National Freshman Honor Society (top 10% of rising sophomores) September 2013

## Scientific Presentations

***Selected Oral Presentations***

**Multiscale simulations examining glycan shield effects on drug binding to influenza neuraminidase**
*Authors: **Seitz, C.**, Casalino, L., Konecny, R., Huber, G., R.E. Amaro, McCammon, J.A.*

- Five presentations, 2018-2021

**Why Do Enolate Anions Favor O-Alkylation in the Gas Phase? The Roles of Resonance and Inductive Effects in the Gas-Phase $S_N2$ Reaction between the Acetaldehyde Enolate Anion and Methyl Fluoride**
*Authors: **Seitz, C.G.**, Zhang, H., Mo, Y., Karty, J.*

- Five presentations (one invited talk), 2015-2016

**The predicted ensemble of 3 dimensional structures for human olfactory receptors**
*Authors: **Seitz, C.G.**, Lebby, M., Arun, N., Zhou, D., Gu, D., Kim, S.-K., Goddard, III, W.A.*

- Three presentations, 2015-2016

**Multifunctional polyurethane hydrogels for biomedical applications**
*Authors: **Seitz, C.G.**, Nguyen-Kim, M.-T., Borghs, J., Wallenborn, J., Böker, A.*

- Five presentations, 2014-2016

***Poster Presentations***

**Multiscale simulations examining glycan shield effects on drug binding to influenza neuraminidase**
*Authors: **Seitz, C.**, Casalino, L., Konecny, R., Huber, G., R.E. Amaro, McCammon, J.A.*

- Four presentations, 2018-2021

**Why Do Enolate Anions Favor O-Alkylation in the Gas Phase? The Roles of Resonance and Inductive Effects in the Gas-Phase $S_N2$ Reaction between the Acetaldehyde Enolate Anion and Methyl Fluoride**
*Authors: **Seitz, C.G.**, Zhang, H., Mo, Y., Karty, J.*

- Five presentations, 2014-2016

**The predicted ensemble of 3 dimensional structures for human olfactory receptors**
*Authors: **Seitz, C.G.**, Lebby, M., Arun, N., Zhou, D., Gu, D., Kim, S.-K., Goddard, III, W.A.*

- Two presentations, 2015-2016

**Multifunctional polyurethane hydrogels for biomedical applications**
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- Five presentations, 2014-2016

## Teaching experience

**Teaching assistant, General Chemistry III lecture** March 2017 – present
*Department of Chemistry and Biochemistry, University of California, San Diego*

- Used research-based interactive learning techniques to teach general chemistry concepts
- Graded project assignments, proctored exams and explained material in office hours and via email

**Teaching assistant, General Chemistry Lab** September 2016 – March 2017
*Department of Chemistry and Biochemistry, University of California, San Diego*

- Taught concepts and supervised general lab technique
- Fall 2016 TA Excellence Award (UCSD), recognizing excellence in teaching

## Technical skills and languages

- Experience working in Python, Bash, Gaussian, Amber, NAMD, MDTraj, CPPTraj, PyEmma, Schrodinger Glide, Schrodinger Maestro, Jupyter Notebooks, BrownDye, Wolfram Mathematica, SAS
- French (advanced conversational proficiency), German (beginning conversational proficiency)

## References

**J. Andrew McCammon**, Distinguished Professor of Chemistry and Biochemistry
Joseph E. Mayer Chair of Theoretical Chemistry

Distinguished Professor of Pharmacology
University of California, San Diego, 858-534-2905, jmccammon@ucsd.edu

**Rommie Amaro**, Professor and Shuler Scholar, Chemistry and Biochemistry
Director, National Biomedical Computation Resource
University of California, San Diego, 858-534-9629, ramaro@ucsd.edu

**William A. Goddard, III**, Charles & Mary Ferkel Professor of Chemistry, Materials Science & Applied Physics
Director, Materials and Process Simulation Center
California Institute of Technology, Pasadena, 626-395-2731, wag@wag.caltech.edu

**Joel Karty**, Professor of Chemistry
Elon University, 336-278-6267, jkarty@elon.edu