Christian Seitz

Employment

University of Chicago, Chicago, IL, USA — February 2023 – Present
Postdoctoral Researcher, Computer Science department

Argonne National Laboratory, Lemont, IL, USA (joint appointment) — February 2023 - Present
Postdoctoral Researcher, Data Science and Learning division

Education

University of California, San Diego (UCSD), La Jolla, CA, USA — November 2022
PhD in Biochemistry & Biophysics, specialization in Multiscale Biology

Elon University, Elon, NC, USA — May 2016
Bachelor of Science in Chemistry, *Cum Laude*

Research Interests

Computational methods are increasing their power to transform our lives, the technology we use, and many areas of research. I am interested in exploiting this expanding power to glue together my background in chemistry with my desire to use biology to tackle problems in global health, either through basic or applied research. A key focus of my research is linking together different scales and disciplines. A single small molecule can be discretely examined through quantum mechanics, or millions can be tested as potential drug inhibitors through high-throughput virtual screening. Structures of large protein complexes can be predicted through neural networks and diffusion models, giving insights into their biological pathways. Protein dynamics can be seen through molecular dynamics, while accessible timescales can be extended further through techniques such as Markov state models, enhanced-sampling molecular dynamics and elastic network models. In summary, my past work and my future interests involve using a wide variety of techniques to investigate global problems, from gaining a better understanding of the proteins involved all the way through to drug and vaccine development.

Postdoctoral Researcher work, member of the Davis and Ramanathan labs

Synopsis: Predicting and evaluating long timescale simulations of protein-antibody complexes

Although SARS-CoV-2 entered the human population in 2019, its relatives in the *Coronaviridae* viral family have been known to researchers as potential pandemic agents for some time. Similarly, Lassa virus and Nipah virus are thought to have pandemic potential. My work utilizes recent advances in the structure prediction of protein complexes as a starting point for long timescale molecular dynamics simulations studying antibody recognition in Lassa and Nipah, with the goal of developing a vaccine for these two viruses. Much community work has been done evaluating the initial, static outputs of different structure prediction programs; what is less understood is how these programs differ, or do not differ, under longer timescale simulations. On a fundamental level, my work also aims to characterize how structure prediction programs fare under protein dynamics that much of the biophysical community uses.

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. *In revisions at Cell CHEM*

Naticchia, M. R., Verespy, S., Kozirovsky, D., **Seitz, C.**, Gaieb, Z., Timm, B., Follmar, J., Huang, M. L., Amaro, R., Godula, K. Chemical Inhibition of Heparan Sulfate Biosynthesis Enables Transient Glycocalyx Editing to Control Stem Cell Signaling and Differentiation. *Submitted to Nature Communications*

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 Communications*

Young, M. A., Rees, S. D., **Seitz, C.,** Zaramela, L., Khera, H., Zengler, K., Amaro, R., Chang, G. Molecular and structural basis of sialidase substrate specificity. *Submitted to PLoS One*

Seitz, C.*, Ahn, S.-H.*, Wei, H.*, Kyte, M.*, Cook, G. M., Krause, K. L., McCammon, J. A. Targeting Tuberculosis: Novel Scaffolds for Inhibiting Cytochrome *bd* Oxidase. *J. Chem. Inf. Model.*, **2024**, *64*, (13). **DOI:** 10.1021/acs.jcim.4c00344

Lopez, B. N. K., Ceciliato, P. H. O., Takahashi, Y., Rangel, F. J., Salem, E. A., Kernig, K., Chow, K., Zhang, L., Sidhom, M., **Seitz, C.**, Zheng, T., Sibout, R., Laudencia-Chingcuanco, D. L., Woods, D. P., McCammon, J. A., Vogel, J. P., Schroeder, J. I. CO_2 response screen in grass *Brachypodium* reveals the key role of a MAP kinase in CO_2-triggered stomatal closure. *Plant Phys.*, **2024**, *196*, (1). **DOI:** 10.1093/plphys/kiae262

Kim, J., Shivkumar, A., Norimoto, M., Castro-Lingl, S., **Seitz, C.**, Amaro, R., Gonias, S. L., Yang, J., Campana, W. M. Binding and activation of LRP1-dependent cell signaling in Schwann cells using a peptide derived from the hemopexin domain of MMP-9. *Biochem.*, **2024**, *63*, (6). **DOI:** 10.1021/acs.biochem.3c00705

Seitz, C., Deveci, İ., McCammon, J.A. Glycosylation and Crowded Membrane Effects on Influenza Neuraminidase Stability and Dynamics. *J. Phys. Chem. Lett.*, **2023**, *14*. **DOI:** 10.1021/acs.jpclett.3c02524

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. *ACS Cent. Sci.,* **2022**, *8*, (12). **DOI:** 10.1021/acscentsci.2c00981

Takahashi, Y., Bosmans, K., Hsu, P.-K., Paul, K., Yeh, C.-Y., Wang, Y.-S., Yarmolinsky, D., Sierla, M., Vahisalu, T., **Seitz, C.,** McCammon, J.A., Kangasjarvi, J., Kollist, H., Zhang, L., Trac, T., Schroeder, J.I. Stomatal CO_2/bicarbonate Sensor Consists of Two Interacting Protein Kinases, Raf-like HT1 and non-kinase-activity requiring MPK12/MPK4. *Sci. Adv.,* **2022**, *8*, (49). **DOI:** 10.1126/sciadv.abq616

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

Letters to a Pre-Scientist, USA August 2023 – Present
Participant

- National program pairing middle-schoolers with professional scientists
- Write letters answering questions and explaining the life of a scientist

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

- Anton 2 research allocation (co-investigator) November 2023
- CCG Excellence Award for Graduate Students – one of five winners at ACS Spring 2023 March 2023
- 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., Amaro, R.E., 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
Authors: ***Seitz, C.G.****, Nguyen-Kim, M.-T., Borghs, J., Wallenborn, J., Böker, A.*

- 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

- Publications using Python, Jupyter Notebooks, Gaussian, Amber, NAMD, GaMD, BrownDye, ProDy, MDTraj, CPPTraj, PyEmma, VMD, MOE
- Experience working in Bash, Schrödinger Maestro, Schrödinger Glide, PyMOL
- French (advanced conversational proficiency), German (beginning conversational proficiency)

References

James Davis, Group Leader
Department of Computer Science
University of Chicago, 630-252-1190, jjdavis@anl.gov

Arvind Ramanathan, Computational Science Leader I
Data Science and Learning Division
Argonne National Laboratory, 630-252-3805, ramanathana@anl.gov

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, Distinguished Professorship in Theoretical and Computational Chemistry
Department of Molecular Biology
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, Associate Professor
Department of Chemistry
Elon University, 336-278-6267, jkarty@elon.edu