

## EDUCATION

Ph.D. student **University of California at Santa Cruz**.  
Graduation Date: June, 2021 (expected).  
GPA: 3.88 out of 4.0  
Computer Science major (from 2016 to 2020)  
Biomolecular Engineering and Bioinformatics major (starting FALL 2020).  
Thesis: Structure-based modeling of peptide/MHC complexes.

M.S., **San José State University**.  
Graduation Date: May, 2015.  
GPA: 3.97 out of 4.0  
Computer Science major.

B.E., **Sri Jayachamarajendra College of Engineering**.  
Graduation Date: June, 2011.  
GPA: 9.34 out of 10.0  
Computer Science major.

## PUBLICATIONS Peer-reviewed Journal Papers

**Nerli, S.**, De Paula, V.S., McShan, A.C., Sgourakis, N.G.. *Backbone-independent NMR resonance assignments of methyl probes in large proteins*. Nature Communications (*in revision*).

**Nerli, S.** and Sgourakis, N.G.. *Structure-based modeling of SARS-CoV-2 peptide/HLA antigens*. Frontiers in Medical Technology and Pharmaceutical Innovation (*in revision*).

De Paula, V.S., Jude, K.M., **Nerli, S.**, Glassman, C.R., Garcia, K.C., Sgourakis, N.G., *Interleukin-2 druggability is modulated by global conformational transitions controlled by a helical capping switch*. PNAS, 2020.

Wei, K.Y., Moschidi, D., Bick, M.J., **Nerli, S.**, McShan, A.C., Carter, L.P., Huang, P.S, Fletcher, D.A., Sgourakis, N.G., Boyken, S.E., Baker, D., *Computational design of closely related proteins that adopt two well-defined but structurally divergent folds*, PNAS, 2020.

Fernandes, J.D., Hinrichs, A.S., Clawson, H., Gonzales, J.N., Lee, B.T., Nassar, L.R., Raney, B.J., Rosenbloom, K.R., **Nerli, S.**, Rao, A.A., Schmelter, D., Zweig, A.S., Lowe, T.M., Ares, M., Corbett-Detig, R., Kent, J.W., Haussler, D., Haeussler, M. *The UCSC SARS-CoV-2 Genome Browser*, Nature Genetics, 2020.

Marceau, A.H.\*, Brison, C.M.\*, **Nerli, S.\***, Arsenault, H.E., McShan, A.C., Chen, E., Lee, H.W., Benanti, J.A., Sgourakis, N.G., Rubin, S.M. *An order-to-disorder structural switch activates the FoxM1 transcription factor*. elife, 2019. \*- authors contributed equally to this work.

**Nerli, S.** and Sgourakis, N.G.. *CS-Rosetta*. Methods in Enzymology, 2019.

Marcos, E., Chidyausiku, T.M., McShan, A.C., Evangelidis, T., **Nerli, S.**, Carter, L., Nivón, L.G., Davis, A., Oberdorfer, G., Tripsianes, K., Sgourakis, N.G., Baker, D.,

*De novo design of a non-local  $\beta$ -sheet protein with high stability and accuracy.* Nature Structural and Molecular Biology, 2018.

**Nerli, S.**, McShan, A.C., Sgourakis, N.G. *Chemical shift-based methods in NMR structure determination.* Progress in Nuclear Magnetic Resonance Spectroscopy. 2018

Evangelidis, T., **Nerli, S.**, Nováček, J., Brereton, A.E., Karplus, P.A., Dotas, R.R., Venditti, V., Sgourakis, N.G., Tripsianes, K. *Automated NMR resonance assignments and structure determination using a minimal set of 4D spectra.* Nature Communications, 2018.

Toor, J.S., Rao, A.A., McShan, A.C., Yarmarkovich, M., **Nerli, S.**, Yamaguchi, K., Madejska, A.A., Nguyen, S., Tripathi, S., Maris, J.M., Salama, S.R., Haussler, D., Sgourakis, N.G. *A recurrent mutation in anaplastic lymphoma kinase with distinct neopeptide conformations.* Frontiers in Immunology, 2018.

### Poster and Oral Presentations

*High-throughput Homology Modeling of Peptide/MHC Complexes.*  
with Nikolaos G. Sgourakis, Assistant Professor. UCSC  
RosettaCon - 2020.  
Seattle, Washington, USA. 2020.

*Helping Rosetta approximate Side-chain Conformational Entropy.*  
with Nikolaos G. Sgourakis, Assistant Professor. UCSC  
RosettaCon - 2019.  
Seattle, Washington, USA. 2019.

*Protein Side-chain Placement as a Constraint Satisfaction Problem.*  
with Nikolaos G. Sgourakis, Assistant Professor. UCSC  
RosettaCon - 2018.  
Seattle, Washington, USA. 2018.

*Maximal Dependence Decomposition Algorithm for Identification of Conserved Motifs.*  
with Anthony Bortolazzo, undergraduate student in Biological Sciences, Dhivya Srinivasan, graduate student in Computer Science, Sami Khuri, Professor and Chair, Department of Computer Science, SJSU, Natalia Khuri, PhD candidate in Biophysics, UCSF.  
26<sup>th</sup> Annual CSU Biotechnology Symposium.  
Santa Clara, California, USA. 2014.

*Towards a Better Understanding of the Unclassified Variants of the BRCA1 gene.*  
with Anthony Bortolazzo, undergraduate student in Biological Sciences, Kiranmayee Dhavala, Vidya Ramprakash, graduate students in MBT Program, Sami Khuri, Professor and Chair, Department of Computer Science, SJSU.  
9<sup>th</sup> Annual Biology and Mathematics in Bay Area Meeting.  
University of California.  
Davis, California, USA. 2014.

*Genome-wide Prediction of Splice Sites using Maximal Dependence Decomposition.*  
with Sami Khuri, Professor and Chair, Department of Computer Science, SJSU.  
AAAS 2015 Annual Meeting.  
San José, California, USA. 2015.

*Genome-wide Prediction of Splice Sites using Maximal Dependence Decomposition.*  
with Sami Khuri, Professor and Chair, Department of Computer Science, SJSU.  
BCATS Symposium, 2015.  
Palo Alto, California, USA. 2015.

*Using Statistical Models to Predict Splice Sites and Cryptic Splice Sites.*  
with Sami Khuri, Professor and Chair, Department of Computer Science, SJSU.  
AAAS, Pacific Division 2015.  
San Francisco, California, USA. 2015.

#### **Master's Thesis**

Santrupti Nerli. Using Hidden Markov Models to Detect DNA Motifs. Master's Thesis,  
San José State University, 2015.

### **AWARDS**

SJSU Research, Scholarship and Creative Activity (RSCA) award. 2013 - 2014.

36<sup>th</sup> Annual SJSU Student Research Competition Winner (US \$750). April 2015.

Second Place Award (US \$250) for oral presentation of *Genome-wide Prediction of Splice Sites using Classification Trees* in Engineering and Computer Science, Session 11, 29<sup>th</sup> CSU Student Research Competition, San Bernardino. May 2015.

### **EXPERIENCE**

**University of California at Santa Cruz.** Santa Cruz, CA.

*Graduate Research Assistant. Sgourakis Lab.* September 2016 - Current.

I am developing computational methods to predict accurate protein structures using sparse experimental data.

**University of California at Santa Cruz.** Santa Cruz, CA.

*Teaching Assistant. CMPS 102, Data structures.* Jan 2017 - March 2017.

**Intuit.** Mountain View, CA.

*Software Engineer. QuickBooks Online.* June 2015 - June 2016.

I developed a software to post feeds for payroll service setup on QuickBooks Online product. In the back-end, I handled triggers for feeds using Java. Further, I developed click tracking in the UI in JavaScript.

**San José State University.** San José, CA.

*Research Assistant. VanHoven Lab .* April 2015 - June 2015.

I worked with biologists at Dr. VanHoven's lab to develop plugins for ImageJ, to automate the workflow of image analysis of *C.elegans* worm.

**San José State University.** San José, CA.

*Research Assistant. Dr. Sami Khuri's Group.* September 2013 - May 2015.

I worked with Dr. Khuri in developing statistical methods to predict splice sites and cryptic splice sites in a human genome. The methods are developed in C and Java.

**San José State University.** San José, CA.

*Teaching Associate. Department of Computer Science.* January 2015 - May 2015.

I taught a 3 unit undergraduate course, CS49J-Programming in Java.

**Symantec Corporation.** Mountain View, CA.

*Intern. Endpoint Engineering Organization.* June 2014 - May 2015.

I developed a feature in C++ to support removable disk encryption to the existing whole disk encryption product. This feature is used as a recovery mechanism in case of driver failures.

**San José State University.** San José, CA.

*Research Assistant. Wilkinson Lab.* August 2014 - December 2014.

I worked with Dr. Wilkinson's lab in developing a Python script to analyze vibration data obtained by recording the nerve firing properties due to inflammation and Obesity in male and female mice.