Education Duke University

Sept. 2016 - Present Ph.D. Candidate, Computational Biology & Bioinformatics

GPA: 4.0/4.0

Dartmouth College

June 2014 B.A., Biomedical Engineering with Honors

Minor, Computer Science GPA: 3.65/4.0 - Cum Laude

Research

Sept. 2016 - Present

Donald Lab, Duke University Ph.D. Candidate, Durham, NC

Dr. Bruce R. Donald, Advisor

I develop provable algorithms to compute the partition function and energy landscape of a protein conformation ensemble. I apply these algorithms to design protein therapeutics and investigate the structural biology of peptide binding, antibiotic resistance, and antibody:antigen interactions.

GENIE Project, Howard Hughes Medical Institute

July 2014 - July 2016 Research Technician, Ashburn, VA

Dr. Douglas Kim, Program Scientist; Dr. Eric Schreiter, Group Leader

Responsible for mutagenesis and high-throughput screening of genetically encoded calcium indicator (GECI) variants. Improved activity of CaMPARI, a novel calcium-dependent green to red photocon-

vertible fluorescent protein.

Higgs Lab, Geisel School of Medicine

Nov. 2010 - June 2014 Undergraduate Researcher, Hanover, NH

Dr. Henry N. Higgs, Principal Investigator

My honors thesis, Examination of the Bioengineering of Polarized Microstructures, characterized the localization and behavior of a mammalian cytoskeleton regulatory protein, FMNL3. Research included limited alanine scanning of putative binding sites and fluorescence microscopy.

US Dept. of Energy, Lawrence Berkeley National Laboratory

Aug. - Dec. 2012 Science Undergraduate Laboratory Intern, Berkeley, CA

Dr. Priscilla Cooper, Principal Investigator; Dr. Kelly Trego, Mentor

My independent project, *Transcriptional Regulation of XPG in the DNA Damage Response*, evaluated putative transcription factors of XPG, a double-stranded break DNA repair protein. I inhibited TFs in cultured human cells and evaluated the levels of XPG via qRT-PCR and Western blotting.

Awards and Fellowships

Teaching Assistant Award - Duke University Dept. of Computer Science, 2020

Poster Award - Duke University Dept. of Biochemistry, 2019

RECOMB Travel Fellowship Award - NSF, 2019

James B. Duke Fellowship - Duke University, 2016 - 2020

Tau Beta Pi Engineering Honors Society - Dartmouth College, 2014

Junior Research Scholarship - Dartmouth College, 2013 Sophomore Science Scholarship - Dartmouth College, 2012

Technical Skills

Algorithm Development, Java, Python, MATLAB, LATEX, Unix, Protein Biochemistry, Automated Liquid Handling, Fluorescent Microscopy, Tissue Culture, PCR, SDS-PAGE

Publications

Lowegard, A. U., Frenkel, M. S., Holt, G. T., Jou, J. D., Ojewole, A. A. & Donald, B. R. Novel, provable algorithms for efficient ensemble-based computational protein design and their application to the redesign of the c-Raf-RBD:KRas protein-protein interface. *PLOS Computational Biology* **16** (ed Dunbrack, R. L.) e1007447. ISSN: 1553-7358 (June 2020).

Jou, J. D., Holt, G. T., Lowegard, A. U. & Donald, B. R. Minimization-Aware Recursive K*: A Novel, Provable Algorithm that Accelerates Ensemble-Based Protein Design and Provably Approximates the Energy Landscape. *Journal of Computational Biology* **27.** PMID: 31855059, 550–564 (2020).

Holt, G. T., Jou, J. D., Gill, N. P., Lowegard, A. U., Martin, J. W., Madden, D. R., et al. Computational analysis of energy landscapes reveals dynamic features that contribute to binding of inhibitors to CFTR-associated ligand. *The Journal of Physical Chemistry B* **123**, 10441–10455 (2019).

Reeve, S. M., Si, D., Krucinska, J., Yan, Y., Viswanathan, K., Wang, S., et al. Toward Broad Spectrum Dihydrofolate Reductase Inhibitors Targeting Trimethoprim Resistant Enzymes Identified in Clinical Isolates of Methicillin Resistant Staphylococcus aureus. ACS Infectious Diseases 5. PMID: 31565920, 1896–1906 (2019).

Moeyaert, B., Holt, G., Madangopal, R., Perez-Alvarez, A., Fearey, B. C., Trojanowski, N. F., et al. Improved methods for marking active neuron populations. *Nature Communications* 9, 4440 (2018).

Hallen, M. A., Martin, J. W., Ojewole, A., Jou, J. D., Lowegard, A. U., Frenkel, M. S., et al. OSPREY 3.0: Open-source protein redesign for you, with powerful new features. *Journal of Computational Chemistry* **39**, 2494–2507 (2018).

de Juan-Sanz, J., Holt, G. T., Schreiter, E. R., de Juan, F., Kim, D. S. & Ryan, T. A. Axonal Endoplasmic Reticulum Ca2+ Content Controls Release Probability in CNS Nerve Terminals. *Neuron* **93**, 867–881.e6. ISSN: 0896-6273 (2017).

Dana, H. et al. Sensitive red protein calcium indicators for imaging neural activity. eLife $\bf 5$ (ed Häusser, M.) e12727. ISSN: 2050-084X (Mar. 2016).

Henderson, M. J., Baldwin, H. A., Werley, C. A., Boccardo, S., Whitaker, L. R., Yan, X., et al. A Low Affinity GCaMP3 Variant (GCaMPer) for Imaging the Endoplasmic Reticulum Calcium Store. *PLOS ONE* **10**, 1–17 (Oct. 2015).