

# Mark Hallen

## Research Assistant Professor

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## Education

**PhD in Computer Science, May 2016, Duke University**, Durham, NC, with a certificate in Structural Biology and Biophysics. **Advisor: Bruce Donald**. Thesis topic: Protein and drug design algorithms using improved biophysical modeling. GPA: 3.97

BS (summa cum laude, Phi Beta Kappa) in Chemistry (ACS certified) and Mathematics (with distinction; senior thesis: "Improving the Accuracy and Scope of Quantitative FRAP analysis"), May 2009, Duke University.

Undergraduate GPA: 3.94

High school diploma, May 2006, Cary Academy, Cary, NC.

## Honors and Awards

- Dolores Zohrab Liebmann fellow, 2015
- Kamin poster award, Duke biochemistry departmental retreat, 2014
- PhRMA Informatics fellow, 2012
- National Defense Science and Engineering Graduate Fellow, 2009
- James B. Duke fellow, 2009
- Julia Dale Prize, Duke math department, 2009
- Goldwater scholar, 2008
- PRUV fellow (for summer research in math at Duke), 2008
- National Merit Scholarship, 2006
- National Chemistry Olympiad finalist; attended two-week study and US team selection camp at the US Air Force Academy, Colorado Springs, CO, June 2006
- USA Mathematical Olympiad qualifier, 2006
- USA Biology Olympiad semifinalist, 2004
- 5th in US (1st in NC) on American Mathematics Competition (AMC) (10A division), 2004

## Languages

- Java
  - Wrote large portion of OSPREY protein design software; leading ongoing refactoring effort
- Other programming languages: Python, C++, HTML, MATLAB
- Natural languages: English, Spanish, French, Russian

## Professional Experience

- PhD thesis research performed with Dr. Bruce Donald; also performed research with Drs. Lingchong You, David Beratan, and Michael Fitzgerald in the first year of graduate school.
- Intern, Vaccine Research Center (National Institutes of Health), May-August 2014. Advisors: Drs. Peter Kwong and Ivelin Georgiev.
- Undergraduate researcher, Dr. Sharyn Endow's lab, Duke Dept. of Cell Biology, December 2006-May 2009
  - Worked on microtubule motors, especially data analysis and modeling for FRAP (fluorescence recovery after photobleaching) and other experiments.
- Pre-undergraduate researcher, Dr. Nina Allen's and Dr. Hans Hallen's labs, NC State Univ., summers 2004-2006
- Undergraduate assistant to Director of Academic Support Programs, Duke Univ. Graduate School, September 2006-April 2007

## Activities

- Program committee member for ISMB 2017
- Reviewer for Journal of Chemical Theory and Computation and PLoS Computational Biology
- Duke math club, 2006-2009
  - Putnam score of 26 (top 12%), Dec. 2008

## Publications

1. **Hallen, Mark A.** and Bruce R. Donald. "CATS (Coordinates of Atoms by Taylor Series): Protein design with backbone flexibility in all locally feasible directions." *Bioinformatics* 2017;33(14): i5-i12.
2. **Hallen, Mark A.**, Jonathan D. Jou, and Bruce R. Donald. "LUTE (Local Unpruned Tuple Expansion): Accurate continuously flexible protein design with general energy functions and rigid-rotamer-like efficiency." *Research in Computational Molecular Biology (RECOMB) 2016 proceedings*, volume 9649 of *Lecture Notes in Computer Science*, pp. 122–136. Springer International Publishing, 2016.
  - Journal version: **Hallen, Mark A.**, Jonathan D. Jou, and Bruce R. Donald. "LUTE (Local Unpruned Tuple Expansion): Accurate continuously flexible protein design with general energy functions and rigid-rotamer-like efficiency." *Journal of Computational Biology* 2017;24(6):536-546.
3. Pan, Yuchao, Yuxi Dong, Jingtian Zhou, **Mark Hallen**, Bruce R. Donald, Jianyang Zeng, and Wei Xu. "cOSPREY: A cloud-based distributed algorithm for large-scale computational protein design." *Journal of Computational Biology* 2016;23(9):737-749.
4. **Hallen, Mark A.**, Pablo Gainza, and Bruce R. Donald. "Compact representation of continuous energy surfaces for more efficient protein design." *Journal of Chemical Theory and Computation* 2015;11(5):2292-2306.
5. **Hallen, Mark A.** and Bruce R. Donald. "COMETS (Constrained Optimization of Multistate Energies by Tree Search): A provable and efficient algorithm to optimize binding affinity and specificity with respect to sequence." *Research in Computational Molecular Biology (RECOMB) 2015 proceedings*, volume 9029 of *Lecture Notes in Computer Science*, pp. 122–135. Springer International Publishing, 2015.

- Journal version: **Hallen, Mark A.** and Bruce R. Donald. “COMETS (Constrained Optimization of Multistate Energies by Tree Search): A provable and efficient protein design algorithm to optimize binding affinity and specificity with respect to sequence.” *Journal of Computational Biology* 2016;23(5):311-321.
6. Kwon, Young Do, Marie Pancera, Priyamvada Acharya, Ivelin S. Georgiev, Emma T. Crooks, Jason Gorman, M. Gordon Joyce, Miklos Guttman, Xiaochu Ma, Sandeep Narpala, Cinque Soto, Daniel S. Terry, Yongping Yang, Tongqing Zhou, Goran Ahlsen, Robert T. Bailer, Michael Chambers, Gwo-Yu Chuang, Nicole A. Doria-Rose, Aliaksandr Druz, **Mark A. Hallen**, Adam Harned, Tatsiana Kirys, Mark K. Louder, Sijy O’Dell, Gilad Ofek, Keiko Osawa, Madhu Prabhakaran, Mallika Sastry, Guillaume B. E. Stewart-Jones, Jonathan Stuckey, Paul V. Thomas, Tishina Tittley, Constance Williams, Baoshan Zhang, Hong Zhao, Zhou Zhou, Bruce R. Donald, Lawrence K. Lee, Susan Zolla-Pazner, Ulrich Baxa, Arne Schön, Ernesto Freire, Lawrence Shapiro, Kelly K. Lee, James Arthos, James B. Munro, Scott C. Blanchard, Walter Mothes, James M. Binley, Adrian B. McDermott, John R. Mascola, and Peter D. Kwong. “Crystal structure, conformational fixation and entry-related interactions of mature ligand-free HIV-1 Env.” *Nature Structural and Molecular Biology* 2015;22:522-531.
  7. Roberts, Kyle E., Pablo Gainza, **Mark A. Hallen**, and Bruce R. Donald. “Fast gap-free enumeration of conformations and sequences for protein design.” *Proteins* 2015;83(10):1859-1877.
  8. **Hallen, Mark A.**, Daniel A. Keedy, and Bruce R. Donald. “Dead-End Elimination with Perturbations (“DEEPer”): A provable protein design algorithm with continuous sidechain and backbone flexibility.” *Proteins* 2013;81(1):18-39.
  9. Liu, Hong-Lei, **Mark A. Hallen**, and Sharyn A. Endow. “Altered nucleotide-microtubule coupling and increased mechanical output by a kinesin mutant.” *PLoS ONE* 2012;7(10):e47148.
  10. Endow, Sharyn A. and **Mark A. Hallen**. “Anastral spindle assembly and  $\gamma$ -tubulin in *Drosophila* oocytes.” *BMC Cell Biol.* 2011;12:1, doi: 10.1186/1471-2121-12-1.
  11. **Hallen, Mark A.**, Zhang-Yi Liang, and Sharyn A. Endow. “Two-state displacement by the kinesin-14 Ncd stalk.” *Biophys. Chem.* 2011;154(2-3):56-65, doi:10.1016/j.bpc.2011.01.001.
  12. Xu, Ying, Irene N. Falk, **Mark A. Hallen**, and Michael C. Fitzgerald. “Mass spectrometry- and lysine amidation-based protocol for thermodynamic analysis of protein folding and ligand binding interactions.” *Anal. Chem.* 2011;83(9):3555-3562.
  13. **Hallen, Mark**, Bochong Li, Yu Tanouchi, Cheemeng Tan, Mike West, and Lingchong You. “Computation of steady-state probability distributions in stochastic models of cellular networks.” *PLoS Comp. Biol.* 2011;7(10):e1002209.
  14. **Hallen, Mark A.**, and Anita T. Layton. “Expanding the scope of quantitative FRAP analysis.” *J. Theor. Biol.* 2010;262(2):295-305.
  15. Liang, Zhang-Yi, **Mark A. Hallen**, and Sharyn A. Endow. “Mature *Drosophila* meiosis I spindles comprise microtubules of mixed polarity.” *Curr. Biol.* 2009;19(2):163-168.
  16. **Hallen, Mark A.**, and Sharyn A. Endow. “Anastral spindle assembly: a mathematical model.” *Biophys. J.* 2009;97(8):2191-2201.
  17. **Hallen, Mark A.** and Hans D. Hallen. “Synthesis of carboxylic acid monolayers by ozonolysis of 10-undecenyltrichlorosilane SAMs.” *J. Phys. Chem. C* 2008;112(6):2086-2090.
  18. **Hallen, Mark A.**, Jianghai Ho, Christine D. Yankel, and Sharyn A. Endow. “Fluorescence recovery kinetic analysis of  $\gamma$ -tubulin binding to the mitotic spindle.” *Biophys. J.* 2008;95(6):3048-3058.
  19. **Hallen, Mark A.**, Zhang-Yi Liang, and Sharyn A. Endow. “Ncd motor binding and transport in the spindle.” *J. Cell Sci.* 2008;121:3834-3841.

20. Zou, Jianwei, **Mark A. Hallen**, Christine D. Yankel, and Sharyn A. Endow. "A microtubule-destabilizing kinesin motor regulates spindle length and anchoring in oocytes." *J. Cell Biol.* 2008;183(3):459-466.
- Poster presentations:
    1. **Hallen, Mark A.**, Jonathan D. Jou, and Bruce R. Donald. "LUTE (Local Unpruned Tuple Expansion): Accurate continuously flexible protein design with general energy functions and rigid-rotamer-like efficiency." Poster at the Biophysical Society Annual Meeting, Feb. 11-15, 2017.
    2. **Hallen, Mark A.**, Pablo Gainza, and Bruce R. Donald. "Energy as Polynomials in Internal Coordinates (EPIC): A compact representation of continuous energy surfaces for more efficient protein design." Poster at the 2014 Duke biochemistry research symposium.
    3. **Hallen, Mark A.**, Priyamvada Acharya, M. Gordon Joyce, Guillaume B. E. Stewart-Jones, Tongqing Zhou, Lei Chen, Rebecca Lynch, John R. Mascola, Peter D. Kwong, Ivelin S. Georgiev, and Bruce R. Donald. "Computational design of probes and antibodies using EPIC and COMETS." Poster at the 2014 Duke biochemistry retreat.
    4. Liu, Hong-Lei, **Mark A. Hallen**, and Sharyn A. Endow "Increased mechanical output by a kinesin mutant." Poster at the Biophysical Society Annual Meeting, Feb. 2-6, 2013.
    5. **Hallen, Mark A.**, Daniel A. Keedy, and Bruce R. Donald. "A provable protein design algorithm with continuous sidechain and backbone flexibility." Poster at the Biophysical Society Annual Meeting, Feb. 2-6, 2013.
    6. **Hallen, Mark A.**, Daniel A. Keedy, and Bruce R. Donald. "Protein design with more realistic continuous flexibility." Poster at the 2012 Duke Biochemistry retreat.
    7. **Hallen, Mark A.**, Daniel A. Keedy, and Bruce R. Donald. "Dead-End Elimination with Perturbations ('DEEPer'): A provable protein design algorithm with continuous sidechain and backbone flexibility." Poster at the 2011 Duke Biochemistry retreat.
    8. **Hallen, Mark**, Patrick DeArmond, Erin Strickland, Jiyong Hong, and Michael Fitzgerald. "Discovery of manassantin A protein targets using a highly multiplexed mass spectrometry-based screening assay." Poster at the 2010 Duke Biochemistry retreat.
    9. **Hallen, Mark A.**, Zhang-Yi Liang, and Sharyn A. Endow. "Microtubule binding and rotation of the kinesin-14 stalk." Poster at the Biophysical Society Annual Meeting, Mar. 3, 2009.
    10. **Hallen, Mark A.**, Zhang-Yi Liang, and Sharyn A. Endow. "Stalk rotation and steps for a kinesin-14 motor." Poster at the ASCB Annual Meeting, Dec. 8, 2009.
    11. **Hallen, Mark A.**, and Hans D. Hallen. "Carboxylate surface functionalization via ozonolysis of vinyl-terminated self-assembled monolayers." Poster at the ACS Colloid and Surface Science Symposium, Jun. 15-18, 2008.
    12. Liang, Zhang-Yi, **Mark A. Hallen**, and Sharyn A. Endow. "Microtubule growth in an anastral spindle from both the chromosomes and poles." Poster at the ASCB Annual Meeting, Dec. 16, 2008.
    13. **Hallen, Mark A.**, Zhang-Yi Liang, and Sharyn A. Endow. "Ncd motor binding and transport in the spindle." Poster at the ASCB Annual Meeting, Dec. 17, 2008.

14. **Hallen, Mark A.**, Jianghai Ho, Christine D. Yankel, and Sharyn A. Endow. " $\gamma$ -Tubulin binds transiently to mitotic spindles, differing from centrosomes." Poster at the American Society for Cell Biology Annual Meeting, Dec. 3, 2007.