

B. Scott Perrin, Jr.

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Laboratory of Computational Biology
National Heart, Lung, and Blood Institute
National Institutes of Health
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Education

- 2011 **Ph.D., Chemistry, Georgetown University**
Advisor: Toshiko Ichiye
Thesis: *Electron Transfer and Assembly of FeS Proteins*
- 2005 **B.S., Chemistry, University of Connecticut**
Advisor: Challa V. Kumar
Thesis: *Computational Modeling of Zinc Binding to Proteins*

Research Experience

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|----------------|---------------------------------|---------------------------|----------------------------|
| 2011 – Present | IRTA Postdoctoral Fellow | NHLBI, NIH | Advisor: Richard W. Pastor |
| Summer 2011 | IRTA Predoctoral Fellow | NHLBI, NIH | Advisor: Bernard R. Brooks |
| 2005 – 2011 | Research Assistant | Georgetown University | Advisor: Toshiko Ichiye |
| 2004 – 2005 | Intern | Bristol-Myers Squibb | Advisor: Graham Poindexter |
| 2003 – 2005 | Undergraduate Researcher | University of Connecticut | Advisor: Challa V. Kumar |

Awards & Achievements

- 2016 **Intramural AIDS Research Fellowship**, NIH
- 2016 **Outstanding Fellow Award**, NHLBI, NIH
- 2015 **Orloff Technical Advance Award**, NHLBI, NIH; *For the Development of CHARMMing*
- 2015 **Postbac Distinguished Mentor Award**, Office of Intramural Education & Training, NIH
- 2014, 2015 **Two 100,000 Node-hour Allocations on the Anton Supercomputer**; *Co-wrote applications*
- 2011 – Present **Implemented and Maintain Reduction Potential Calculations into CHARMMing**
- 2008 – 2009 **President**, Graduate Student Organization of Chemistry, Georgetown University
- 2006 **Espenscheid Fellowship**, Georgetown University
- 2005 **Roland Ward Thesis Award**, University of Connecticut
- 2004 **CBIA/Pfizer Fellowship**, University of Connecticut

Teaching Experience

- 2009 – Present **Chemistry 573: Computational Methods for Biological Macromolecules**
Biannually guest lectured two classes, Georgetown University
- Oct 2014 **Chemistry 320: Biophysical Chemistry**
Guest lectured two classes, Hamilton College
- 2006 – 2009 **Tutor**, Organic Chemistry
- 2005 – 2006 **Teaching Assistant**, General Chemistry

Professional Societies & Organizations

- 2006 – Present **Biophysical Society**, Membrane Structure & Assembly Subgroup
- 2004 – Present **American Chemical Society**
- 2013 – 2014 **NIH Entrepreneur and Commercialization Club**
- 2012 – 2014 **Games for Science Interest Group, NIH**

Software / Application Development

Amphipathic Peptide Analysis: Helical Wheel Projections & Charge Prediction
CHARMM Interface and Graphics: Reduction Potential Module

helix.perrinresearch.com
www.charmming.org

Peer Review

Reviewer for the following journals: *Biophysical Journal*, *Journal of Physical Chemistry B*, *Journal of Physical Chemistry Letters*, and *Physical Review E*

Publications

17. R. M. Venable; Ingólfsson, H. I.; Lerner, M. G.; **Perrin Jr., B. S.**; Camley, B. A.; Marrink, S.-J.; Brown, F. L. H.; and Pastor, R. W. Lipid diffusion in bilayers: The Saffman-Delbrück model and periodic boundary conditions. **Under Review.**
16. S. M. Gordon; Pourmousa, M.; Sampson, M.; Sviridov, D; Islam, R.; **Perrin Jr., B. S.**; Kemeh, G.; Pastor, R. W.; and Remaley, A. T. Identification of a Novel Lipid Binding Motif in Apolipoprotein B by the Analysis of Hydrophobic Cluster Domains. *Biochim. Biophys. Acta, Biomembr.* **2017.** 1859, 135-145.
15. **B. S. Perrin Jr.** and Pastor, R. W. Simulations of membrane disrupting peptides I: Alamethicin pore stability and spontaneous insertion. *Biophys. J.* **2016.** 111, 1248-1257.
14. **B. S. Perrin Jr.**; Fu, R.; Cotten, M. L.; and Pastor, R. W. Simulations of membrane disrupting peptides II: AMP Piscidin 1 favors surface defects over pores. *Biophys. J.* **2016.** 111, 1258-1266.
13. M-L. Tan; **Perrin Jr., B. S.**; Niu, S.; Huang, Q.; and Ichiye T. Protein dynamics and the all-ferrous [Fe₄S₄] cluster in the Nitrogenase Iron Protein. *Protein Sci.* **2016.** 25, 12-18.
12. **B. S. Perrin Jr.**, Sodt, A. J.; Cotten, M. L.; and Pastor, R. W. The curvature induction of surface-bound antimicrobial peptides piscidin 1 and piscidin 3 varies with lipid chain length. *J. Membr. Biol.* **2015.** 248, 455-467.
11. **B. S. Perrin Jr.**, Miller, B. T.; Schalk, V.; Woodcock, H. L.; Brooks, B. R.; and Ichiye, T. Web-based computational chemistry education with CHARMMing III: reduction potentials of electron transfer proteins. *PLoS Comp. Biol.* **2014.** 10: e1003739.
10. **B. S. Perrin Jr.**, Tian, Y.; Fu, R.; Grant, C. V.; Chekmenev, E. Y.; Wieczorek, W. E.; Dao, A. E.; Hayden, R. M.; Burzynski, C. M.; Venable, R. M.; Sharma, M.; Opella, S. J.; Pastor, R. W.; and Cotten, M. L. High-resolution structures and orientations of antimicrobial peptides piscidin 1 and piscidin 3 in fluid bilayers reveal tilting, kinking, and bilayer immersion. *J. Am. Chem. Soc.* **2014.** 136, 3491-3504. [Cover]
9. **B. S. Perrin Jr.**; Pastor, R. W.; and Cotten, M. Combining NMR spectroscopic measurements and molecular dynamics simulations to determine the orientation of amphipathic peptides in lipid bilayers. *Advances in Biological Solid State NMR* (Separovic, F. ed.), Royal Society of Chemistry, Cambridge. **2014.** p 18-35.
8. **B. S. Perrin Jr.** and Ichiye, T. Identifying sequence determinants of reduction potentials of metalloproteins. *J. Biol. Inorg. Chem.* **2013.** 6, 599-608.
7. **B. S. Perrin Jr.** and Ichiye, T. Identifying residues that cause pH-dependent reduction potentials. *Biochemistry.* **2013.** 52, 3022-3024.
6. **B. S. Perrin Jr.** and Ichiye, T. Characterizing protein environmental effects on reduction potentials of metalloproteins. *J. Biol. Inorg. Chem.* **2013.** 18, 103-110.
5. **B. S. Perrin Jr.**; Niu, S.; and Ichiye, T. Calculating standard reduction potentials of metalloproteins. *J. Comp. Chem.* **2013.** 34, 576-582.
4. **B. S. Perrin Jr.** and Ichiye, T. Fold versus sequence effects on the driving force for protein mediated electron transfer. *Proteins.* **2010.** 78, 2798-2808.

3. M.R. Duff; Tan, W.B.; Bhambhani, A.; **Perrin Jr., B.S.**; Thota, J.; Rogers, A.; and Kumar, C.V. Contributions of hydroxyethyl groups to the DNA binding affinities of anthracene probes. *J. Phys. Chem., B.* **2006**, *110*, 20693-20701.
2. N. K. Modukuru; Snow, K. J.; **Perrin Jr., B. S.**; Thota, J.; and Kumar, C. V. The contributions of a long side chain to the binding affinity of an anthracene derivative to DNA. *J. Phys. Chem., B.* **2005**, *109*, 11810-11818.
1. N. K. Modukuru; Snow, K. J.; **Perrin Jr., B. S.**; Bhambhani, A.; Duff, M.; and Kumar, C. V. Tuning the DNA binding modes of an anthracene derivative with salt. *J. Photochem. Photobiol.* **2005**, *177*, 43-54.

Workshops

Introduction to Grant Writing , NHLBI/NIH, Bethesda, MD	August 2015
Writing and Publishing a Scientific Paper Workshop , NIH, Bethesda, MD	October 2012
Advances in Biomolecular Modeling and Simulations using CHARMM , Washington, DC	May 2012
Research Frontiers in Bioinspired Energy , Washington, DC	January 2011
Q-Chem Workshop , Washington, DC	August 2009
Open Science Grid Workshop , Washington, DC	April 2008
TeraGrid Planning Workshop , Chicago, IL	August 2007

Posters and Presentations

Biophysical Society 60th Annual Meeting ; Talk <i>The Disruptive State Of The Membrane Active Antimicrobial Peptide Piscidin 1 Investigated By Multi-μs All-atom Simulations And Solid-State NMR: Surface Defects Are Favored Over Stable Pores</i>	February 2016
Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment ; Talk <i>Membrane Disruption by the Antimicrobial Peptide Piscidin</i>	July 2015
Biophysical Society 59th Annual Meeting ; Talk <i>The Curvature Induction by Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3 Varies with Lipid Chain Length</i>	February 2015
Department of Chemistry Seminar, Hamilton College ; Seminar <i>Curvature Induction by the Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3</i>	Oct 2014
Computation Chemistry Gordon Research Conference ; Poster <i>The Curvature Induction of Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3</i>	July 2014
Student/Postdoc Computational/Theory Washington/Baltimore Local Symposium ; Talk <i>Membrane Deformation by the Antimicrobial Peptides Piscidin 1 and Piscidin 3</i>	June 2014
Biophysical Society 58th Annual Meeting ; Poster <i>Antimicrobial Peptides Piscidins Kink at a Central Glycine to Maximize their Hydrophobic Moments</i>	February 2014
Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment ; Talk <i>Simulations of the Antimicrobial Peptide Piscidin</i>	July 2013
Biophysical Society 57th Annual Meeting ; Poster <i>All-Atom Molecular Dynamic Simulations of Piscidin 1 and Piscidin 3 In Lipid Bilayers</i>	February 2013
Iron-sulfur Enzymes Gordon Research Conference ; Poster <i>The Redox Module in CHARMMing: A Web Interface for Calculating the Reduction Potentials of Iron-Sulfur Proteins</i>	June 2012
Iron-sulfur Enzymes Gordon Research Conference ; Poster <i>Characterizing the Protein Environmental Effects on the Reduction Potential</i>	June 2010
American Chemical Society Fall 2009 National Meeting ; Poster <i>Protein Adjustment of Redox Properties of [4Fe-4S] Clusters</i>	August 2009

Iron-sulfur Enzymes Gordon Research Conference; Talk <i>Fold vs. Sequence: Nature's Tuning of Fe-S Protein Reduction Potentials</i>	June 2008
Biophysical Society 51st Annual Meeting; Poster <i>Molecular Dynamics Study on the Role of IscA in Iron-Sulfur Cluster Assembly</i>	March 2007
Iron-sulfur Enzymes Gordon Research Conference; Poster <i>Molecular Dynamics Study on the Role of IscA in Iron-Sulfur Cluster Assembly</i>	June 2006
American Chemical Society Nation Meeting, Poster <i>Computational Modeling of Zinc Binding to Proteins</i>	August 2005