B. Scott Perrin Jr.

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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

2011 – Present	**IRTA Postdoctoral Fellow**	NHLBI, NIH	Advisor: Richard W. Pastor
Summer 2011	**Predoctoral IRTA 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

2015 **Orloff Technical Advance Award**, NHLBI, NIH; *For the Development of CHARMMing*
2015 **Postbac Distinguished Mentor Award**, Office of Intramural Education & Training, NIH
2014 **100,000 Node-hour Allocation on the Anton Supercomputer**; *Co-wrote application*
2011 – Present **Implemented Reduction Potential Calculations into CHARMMing**
2008 – 2009 **President**, Graduate Student Organization of Chemistry
2006 **Espenscheid Fellowship**; *Passed all Phase I Exams on First Attempt*
2004 – 2005 **Roland Ward Thesis Award**; *Best Undergraduate Thesis in Chemistry*
2004 **CBIA/Pfizer Fellowship**; *Undergraduate Summer Research Support*

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**
2004 – Present **American Chemical Society**
2013 – 2014 **NIH Entrepreneur and Commercialization Club**
2012 – 2014 **Games for Science Interest Group, NIH**

Publications

12. **B. S. Perrin Jr**., A. J. Sodt, M. L. Cotten, and R. W. Pastor *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.**, B. T. Miller, V. Schalk, H. L. Woodcock, B. R. Brooks, and T. Ichiye *Web-Based Computational Chemistry Education with CHARMMing III: Reduction Potentials of Electron Transfer Proteins.* PLoS Comp. Biol. **2014.**

10. **B. S. Perrin Jr**., Y. Tian, R. Fu, C. V. Grant, E. Y. Chekmenev, W. E. Wieczorek, A. E. Dao, R. M. Hayden, C. M. Burzynski, R. M. Venable, M. Sharma, S. J. Opella, R. W. Pastor, and M. L. Cotten *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.

9. **B. S. Perrin Jr**., R. W. Pastor, and M. Cotten. *Combining NMR spectroscopic measurements and molecular dynamics simulations to determine the orientation of amphipathic peptides in lipid bilayers*. in Advances in Biological Solid State NMR (Separovic, F. ed.), Royal Society of Chemistry, Cambridge. **2014.** p 18-35.

8. **B. S. Perrin Jr.** and T. Ichiye. *Identifying Sequence Determinants of Reduction Potentials of Metalloproteins*. J. Biol. Inorg. Chem. **2013.** *6,* 599-608.

7. **B. S. Perrin Jr.** and T. Ichiye. *Identifying Residues That Cause pH-dependent Reduction Potentials*. Biochemistry. **2013**. *52,* 3022-3024.

6. **B. S. Perrin Jr.** and T. Ichiye. *Characterizing Protein Environmental Effects on Reduction Potentials of Metalloproteins.* J. Biol. Inorg. Chem. **2013.** *18*, 103-110.

5. **B. S. Perrin Jr.**, S. Niu, and T. Ichiye. *Calculating Standard Reduction Potentials of Metalloproteins*. J. Comp. Chem. **2013.** *34*, 576-582.

4. **B. S. Perrin Jr.** and T. Ichiye. *Fold versus Sequence Effects on the Driving Force for Protein Mediated Electron Transfer*. Proteins. **2010.** *78*, 2798-2808.

3. M.R. Duff, W.B. Tan, A. Bhambhani, **B.S. Perrin Jr.,** J. Thota, A. Rogers, and C.V. Kumar. *Contributions of Hydroxyethyl Groups to the DNA Binding Affinities of Anthracene* Probes. J. Phys. Chem., B. **2006.** *110*, 20693-20701.

2. N. K. Modukuru, K. J. Snow, **B. S. Perrin Jr.**, J. Thota, and C. V. Kumar. *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, K. J. Snow, **B. S. Perrin Jr.**, A. Bhambhani, M. Duff, and C. V. Kumar. *Tuning The DNA Binding Modes of An Anthracene Derivative with Salt*, J. Photochem. Photobiol. **2005.** *177*, 43-54.

Software

Amphipathic Peptide Analysis helix.perrinresearch.com
- Helical Wheel Projections
- pH Dependence

CHARMM INterface and Graphics www.charmming.org
- Reduction Potential Module

Workshops

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

Posters and Presentations

Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment; Talk — July 2015
Membrane Disruption by the Antimicrobial Peptide Piscidin

Biophysical Society 59th Annual Meeting; Talk — February 2015
The Curvature Induction by Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3 Varies with Lipid Chain Length

Department of Chemistry Seminar, Hamilton College; Seminar — Oct 2014
Curvature Induction by the Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3

Computation Chemistry Gordon Research Conference; Poster — July 2014
The Curvature Induction of Surface-Bound Antimicrobial Peptides Piscidin 1 and Piscidin 3

Student/Postdoc Computational/Theory Washington/Baltimore Local Symposium; Talk — June 2014
Membrane Deformation by the Antimicrobial Peptides Piscidin 1 and Piscidin 3

Biophysical Society 58th Annual Meeting; Poster — February 2014
Antimicrobial Peptides Piscidins Kink at a Central Glycine to Maximize their Hydrophobic Moments

Biological Membranes and Membrane Proteins: Challenges for Theory and Experiment; Talk — July 2013
Simulations of the Antimicrobial Peptide Piscidin

Biophysical Society 57th Annual Meeting; Poster — February 2013
All-Atom Molecular Dynamic Simulations of Piscidin 1 and Piscidin 3 In Lipid Bilayers

Iron-sulfur Enzymes Gordon Research Conference; Poster — June 2012
The Redox Module in CHARMMing: A Web Interface for Calculating the Reduction Potentials of Iron-Sulfur Proteins

Iron-sulfur Enzymes Gordon Research Conference; Poster — June 2010
Characterizing the Protein Environmental Effects on the Reduction Potential

American Chemical Society Fall 2009 National Meeting; Poster — August 2009
Protein Adjustment of Redox Properties of [4Fe-4S] Clusters

Iron-sulfur Enzymes Gordon Research Conference; Talk — June 2008
Fold vs. Sequence: Nature's Tuning of Fe-S Protein Reduction Potentials

Biophysical Society 51st Annual Meeting; Poster — March 2007
Molecular Dynamics Study on the Role of IscA in Iron-Sulfur Cluster Assembly

Iron-sulfur Enzymes Gordon Research Conference; Poster — June 2006
Molecular Dynamics Study on the Role of IscA in Iron-Sulfur Cluster Assembly

American Chemical Society Nation Meeting, Poster — August 2005
Computational Modeling of Zinc Binding to Proteins

Peer Reviewer For Scientific Journals

Journal of Physical Chemistry Letters
Journal of Physical Chemistry