# B. Scott Perrin, Jr.

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## Experience

2020-Present **Scientific Software Engineer**, RU Solutions, Pfizer, Inc Supervisor: Tianhong Zhang

- Delivered SARS-COV-2 Mpro mutation surveillance dashboard driven by Real World Data, kinetic data for in-house inhibitors, and structure models. Included access-controlled view of clinical data. [*Elevate award finalist*]
- Developed an ML-module for processing data in the Mpro mutation dashboard.
- PAXLOVID contributions led to 2020/2021 *Vaccine R&D Award* (team)
- Bact. Vaccines & Tech. support led to *WRDM Breakthrough Science & Innovation Prize* nomination (individual).
- Automated several sequencing pipelines for HPC and cloud computing.

2019-2020 **Scientific Software Engineer**, SCAI Biology, Pfizer, Inc Supervisor: Bill Mounts

- Workstream lead and software engineer for the Biology division of R&D analytics and informatics
- Led development of a web portal for managing cytometry experiments, results, and preliminary analysis
- Automated SDK development for omics APIs; collaborated with application leads to align APIs and SDKs
- Integrated metadata management solution with a terminology management service

2017-2019 **Scientific Software Engineer**, R&D Informatics, Pfizer, Inc. Supervisor: Sabine Schefzick

- Scientific software engineer supporting Oncology and Vaccine Research Units
- Member of a global program to build functional genomics pipelines
- Co-Led development of an -omics metadata management application using Agile-like methods
- Coordinated code revisions by three contract developers and feedback from stakeholders and test team
- Built a genome web browser for selecting CRISPR guides based on user-specified targets
- Automated an analysis pipeline for pooled genomic screening experiments

2011 – 2017 **IRTA Postdoctoral Fellow**, NHLBI, NIH Advisor: Richard W. Pastor

- Validated simulated structures of peptides on membrane surface against solid-state NMR results.
- Evaluated ensemble averages of peptide structures (including fluctuation bias) to rule out conformations
- Contrasted spontaneous insertion of pore-forming peptide to a membrane surface-binding peptide
- Mentored two predoctoral IRTA fellows, received Postbac Distinguished Mentor Award
- Built and deployed tools for studying peptide structure at http://helix.perrinresearch.com

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

## 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*

## Skills

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|---|---|
| Programming: | Python (NumPy, SciPy, matplotlib, Scikit-learn, OpenPyXL), Java, Fortran, C, C++ |
| Web Design: | Flask (Python), Django (Python), Spring (Java), JavaScript, React, HTML, CSS, Bootstrap, Highcharts, PrimeReact, Git, GitHub, JIRA, Confluence |
| Database: | MongoDB, MongoEngine, PyMongo, Oracle, SQL, MySQL, Postgres |
| Scientific: | CHARMM, CHARMMing, CHARMM-GUI, NAMD, VMD, PyMOL, APBS, Gaussian, IGV, GIVE |
| IoT: | MQTT, Arduino IDE, various development boards |
| Other: | Agile development, proposal writing, metadata and terminology management |

## Awards & Achievements

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| 2022 | *Nominated*: **Breakthrough Science & Innovation Prize**, Pfizer |
| 2021 | *Finalist*: **Elevate Digital Award**, Individual Award in the Agile Category, Pfizer |
| 2020/2021 | **Vaccine R&D Award**: PAXLOCID Virology EUA Team, Pfizer |
| 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 – 2016 | **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

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

## Professional Societies & Organizations

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| 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 helix.perrinresearch.com
**CHARMM INterface and Graphics:** Reduction Potential Module www.charmming.org

## Workshops & Courses

**AWS Summit New York,** New York, NY — July 2019
**Galien Forum,** New York, NY — October 2017
**Introduction to Grant Writing**, NHLBI/NIH, Bethesda, MD — August 2015
**Research Commercialization Introductory Course**,
National Council of Entrepreneurial Tech Transfer (NCET2), Online — December 2013
**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

## Peer Review

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

## Publications

21. Mary Lynn Baniecki; Rhonda Cardin; Heidi Leister-Tebbe; Yuao Zhu; Shunjie Guan; Craig Hyde; Wen He; Zhenyu Wang; Li Hao; **B. Scott Perrin, Jr.**; Weihang Bao; Phylinda Chan; Bharat Damle; Sandeep Menon; Jennifer Hammond; Annaliesa S. Anderson; Holly Soares; Viral Load Rebound in Placebo and Nirmatrelvir-Ritonavir Treated COVID-19 Patients is not Associated with Recurrence of Severe Disease or Mutations *Submitted*.

20. Jonathan T. Lee, Qingyi Yang, Alexey Gribenko, **B. Scott Perrin Jr.**, Yuao Zhu, Rhonda Cardin, Paul A. Liberator, Annaliesa S. Anderson, Li Hao; Genetic surveillance of SARS-CoV-2 Mpro reveals high sequence and structural conservation prior to the introduction of protease inhibitor Paxlovid *Submitted*.

19. M. Mihailescu, Sorci, M.; Seckute, J.; Silin, V. I.; Hammer, J.; **Perrin Jr., B. S.**; Hernandez, J. I.; Smajic, N.; Shrestha, A.; Bogardus, K. A.; Greenwood, A. I.; Fu, R.; Blazyk, J.;Pastor, R. W.; Nicholson, L. K.; Belford, G.; Cotten, M. L.; Structure and Function in Antimicrobial Piscidins: Histidine Position, Directionality of Membrane Insertion, and pH-dependent Permeabilization *J. Amer. Chem. Soc.* **2019.** *141*, 9837-9853.

18. R. M. Islam; Pourmousa, M.; Sviridov, D.; Gordon, S. M.; Neufeld, E. B.; Freeman, L. A.; **Perrin Jr., B. S.;** Pastor, R. W.; Remaley, A. T.; Structural properties of apolipoprotein AI mimetic peptides that promote ABCA1-dependent cholesterol efflux Scientific Reports. **2018**. *8*, 2956.

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. *J. Phys. Chem. B.* **2017.** *15*, 3443-3457.

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 [$Fe_4S_4$] 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.

## Posters & Presentations

**Antimicrobial Peptides Gordon Research Conference**; Poster February 2017
*Simulations of Membrane-Disrupting Peptides: Pores Versus Surface Binding*

**Biophysical Society 61st Annual Meeting**; Poster, Section Chair February 2017
*Simulations of Membrane-Disrupting Peptides: Pores Versus Surface Binding*

**Biophysical Society 60th Annual Meeting**; Talk February 2016
*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*

**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, Section Chair 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*