Curriculum Vitae

Gregory R. Bowman

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Present Position

2019 - pres	Associate Professor, Department of Biochemistry & Molecular Biophysics, Washington University School of Medicine
2014 - 2019	Assistant Professor, Department of Biochemistry & Molecular Biophysics, Washington University School of Medicine

Education

2002 - 2006	BS, *summa cum laude*, Computer Science, minor Biomedical Engineering, Cornell University, Ithaca, NY
2006 - 2010	PhD, Biophysics, Stanford University, Stanford, CA

Academic Positions / Employment:

2010 - 2011	Berry Postdoctoral Fellow, Stanford University, Stanford, CA
2011 - 2014	Miller Research Fellow, University of California, Berkeley, Berkeley, CA

Honors and Awards

2016-2021	Packard Fellowship
2016-2021	NSF CAREER Award
2013-2018	Burroughs Wellcome Fund Career Award at the Scientific Interface
2011-2014	Miller Research Fellowship
2011	Young Investigator Award, Genome Technology
2010-2011	Berry Postdoctoral Fellowship
2010	Thomas Kuhn Paradigm Shift Award, American Chemical Society
2007-2010	NSF Graduate Research Fellowship
2006	Tau Beta Pi, Cornell University
2006	Merrill Presidential Scholar, Cornell University
2005	Computer Science Department Award for Academic Excellence, Cornell University
2005	Jean Dreyfus Boissevain Undergraduate Scholarship for Excellence in Chemistry, Cornell University

Community Service Contributions

Community Service

2018-pres Director of the Folding@home distributed computing project
2014-pres Outreach to the visually impaired through organizations like the Foundation Fighting Blindness

Professional Societies

2008-pres Biophysical Society

Major Invited Professorships and Lectureships

2020 Pharmaceutical Biophysics Symposium, Biophysical Society
2020 Chemistry Seminar, UIUC, IL
2020 SAGIM drug design community, San Diego
2020 Missouri School for the Bling, MO
2020 National Federation of the Blind, MO
2019 Biophysics Seminar, Johns Hopkins, Baltimore, MD
2019 Chemical Biology Seminar, St. Jude Children's Research Hospital, Memphis, TN
2019 Exploring Cryptic Pockets in Drug Discovery Symposium, ACS National Meeting, Orlando, FL
2019 Molecular Kinetics Workshop, Freie Universitat Berlin, Germany
2019 Chemistry Seminar, Temple University, Philadelphia, PA
2018 Protein Folding Gordon Research Conference, Galveston, TX
2018 Drug Discovery Seminar, Eli Lilly, Indianapolis, IN
2018 Protein Design Seminar, Monsanto, St. Louis, MO
2018 Markov State Models in Drug Discovery Workshop, Novartis, Boston, MA
2018 Platform for Advanced Scientific Computing, Basel, Switzerland
2018 Canadian Chemistry Conference, Edmonton, Canada
2018 Biophysics Seminar, University of Chicago, Chicago, IL
2018 Biochemistry Seminar, University of Wisconsin-Madison, Madison, WI
2018 Chemistry Seminar, Pennsylvania State University, University Park, PA
2018 Biochemistry Seminar, St. Louis University, St. Louis, MO
2018 Midwest Theoretical Chemistry Conference, Chicago, IL
2018 Chemistry Seminar, Illinois Institute of Technology, Chicago, IL
2017 Pharmacology Seminar, Baylor College of Medicine, Houston, TX
2017 Free energy calculations workshop, Telluride, CO
2017 Protein Dynamics & Allostery Platform Session, Biophysical Society, New Orleans, LA
2017 Chemistry Seminar, University of Missouri, St. Louis, MO
2017 Computational Biology Seminar, University of Texas, Southwestern, Dallas, TX
2017 Protein Folding Consortium, University of California, Berkeley, CA
2016 Markov State Models in Drug Discovery Workshop, Novartis, Boston, MA
2016 Pfizer, Boston, MA
2016 UCB Pharmaceuticals, London, United Kingdom
2016 Kings College, London, United Kingdom
2016 Protein Folding Consortium, Washington University in St. Louis, St. Louis, MO
2015 Theoretical Chemistry Institute (TCI) Seminar, University of Wisconsin-Madison, Madison, WI
2015 Free energy calculations workshop, Snowmass, CO
2015 Seminar, Science for Life Lab, Karolinska Institute, Stockholm, Sweden

2015 Center for Biological Systems Engineering Seminar, Washington University in St. Louis, St. Louis, MO
2015 Cell Biology Seminar, Washington University in St. Louis, St. Louis, MO
2015 Biophysical Evenings, Washington University in St. Louis, St. Louis, MO

Prior to beginning my faculty position at Washington University:
2014 Structure, Dynamics, and Allostery in Drug Target Interactions Platform Session, Biophysical Society
2014 Chemistry & Biochemistry Seminar, University of California, Los Angeles
2014 Chemistry Seminar, University of Illinois
2014 Biophysics Seminar, University of Texas, Southwestern
2014 Biochemistry & Molecular Biophysics Seminar, Washington University in St. Louis
2014 Chemistry & Biochemistry Seminar, University of Colorado, Boulder
2014 Chemistry & Biochemistry Seminar, University of Arizona, Tucson
2014 Biochemistry Seminar, Brandeis University
2014 Dr. George W. Raiziss Seminar, University of Pennsylvania
2014 Integrative Biology & Physiology Seminar, University of California, Los Angeles
2014 Endowed Scholars Symposium, University of Texas, Southwestern
2013 Advanced Light Source User Meeting
2013 Computational Medicine Seminar, University of Michigan
2013 Theoretical Chemistry Seminar, Cornell University
2013 Molecular Kinetics Workshop, Freie Universitat Berlin
2013 Enzyme Dynamics Workshop, Telluride Science Research Center
2013 Biophysics Seminar, University of Michigan
2013 Physical Chemistry Seminar, University of California, Berkeley
2013 Physical Chemistry Seminar, University of Pennsylvania
2012 Physical Chemistry Seminar, ETH Zurich
2012 Biophysics Seminar, University of California, San Francisco
2012 Biophysics Seminar, Johns Hopkins University
2012 Protein Folding Workshop, Stony Brook
2012 Folding@home conference, Stanford University
2011 Protein Folding Workshop, University of California, Berkeley
2011 RosettaCon, University of Washington, Seattle
2011 Protein Folding Symposium, Hong Kong University of Science and Technology
2010 Thomas Kuhn Paradigm Shift Award Symposium, American Chemical Society
2010 Protein Folding & Stability Platform Session, Biophysical Society
2010 France-Stanford Exchange Program, Institut Pasteur
2010 Protein Folding Symposium, Notre Dame
2010 GPU Workshop, Lawrence Berkeley National Laboratory
2010 Biomedical Computation at Stanford (BCATS), Stanford University
2010 Stanford High Performance Computing Conference, Stanford University

Bibliography:

A. Original Articles

1. Porter JR, Meller A, Zimmerman MI, Greenberg MJ, **Bowman GR**. Conformational distributions of isolated myosin motor domains encode their mechanochemical properties. ***bioRxiv (accepted at eLife)*** 2020 doi: https://doi.org/10.1101/2019.12.16.878264.

2. Cruz MA, Frederick TE, Singh S, Vithani N, Zimmerman MI, Porter JR, Moeder KE, Amarasinghe GK, **Bowman GR**. Discovery of a cryptic allosteric site in Ebola's 'undruggable' VP35 protein using simulations and experiments. ***bioRxiv*** 2020 doi: https://doi.org/10.1101/2020.02.09.940510.
3. Wang W, Shin W, Zhang B, Choi Y, Yoo J, Zimmerman MI, Frederick TE, **Bowman GR**, Gross ML, Leung DW, Jung JU, Amarasinghe GK. The cap-snatching SFTSV endonuclease domain is an antiviral target. ***Cell Reports*** 2020;30:153-163.
4. Behring JB, Post S, Mooradian AD, Egan MJ, Zimmerman MI, Clements JL, **Bowman GR**, Held JM. Spatial and temporal alterations in protein structure by EGF regulate cryptic cysteine oxidation. ***Sci Signal*** 2020;13:eaay7315.
5. Riehl JR, Zimmerman MI, Singh MF, **Bowman GR**, Ching S. Computing and optimizing over all fixed points of discrete systems on large networks. ***bioRxiv*** 2020 doi: https://doi.org/10.1101/2020.03.04.960724.
6. Brown CA, Hu L, Sun Z, Patel MP, Singh S, Porter JR, Sankaran B, Prasad BVV, **Bowman GR**, Palzkill T. Antagonism between substitutions in b-lactamase explains a path not taken in the evolution of bacterial drug resistance. ***J Biol Chem*** 2020 https://www.jbc.org/cgi/doi/10.1074/jbc.RA119.012489.
7. Porter JR, Moeder KE, Sibbald CA, Zimmerman MI, Hart KM, Greenberg MJ, **Bowman GR**. Cooperative changes in solvent exposure identify cryptic pockets, conformational switches, and allosteric coupling. ***Biophys J*** 2019;116:818-830.
   (selected for a New & Notable: Amaro RE. Will the real cryptic pocket please stand out? Biophys J 2019).
8. Porter JR, Zimmerman MI, **Bowman GR**. Enspara: Modeling molecular ensembles with scalable data structures and parallel computing. ***J Chem Phys*** 2019;150:044108.
9. Behring JB, van der Post, S, Mooradian AD, Egan MJ, Zimmerman MI, Clements JL, **Bowman GR**, Held JM. Spatial and temporal alterations in protein structure by EGF regulate cryptic cysteine oxidation. bioRxiv 2019.
10. Sun X, Singh S, Blumer KJ, **Bowman GR**. Simulation of spontaneous G protein activation reveals a new intermediate driving GDP unbinding. ***eLife*** 2018;7:e38465.
11. Zimmerman MI, Porter JR, Sun X, Silva RR, **Bowman GR**. Choice of adaptive sampling strategy impacts state discovery, transition probabilities, and the apparent mechanism of conformational changes. ***J Chem Theor Comput*** 2018;14:5459-5475.
12. Su Z, Wu C, Shi L, Luthra P, Pintilie GD, Johnson B, Porter JR, Ge P, Chen M, Liu G, Frederick TE, Binning JM, **Bowman GR**, Zhou ZH, Basler CF, Gross ML, Leung DW, Chiu W, Amarasinghe GK. Electron Cryo-microscopy Structure of Ebola Virus Nucleoprotein Reveals a Mechanism for Nucleocapsid-like Assembly. ***Cell*** 2018;172:966-978.
13. Zimmerman MI, Hart KM, Sibbald CA, Frederick TE, Jimah JR, Knoverek CR, Tolia NH, **Bowman GR**. Prediction of New Stabilizing Mutations Based on Mechanistic Insights from Markov State Models. ***ACS Central Science*** 2017;3:1311-1321.
14. Singh S, **Bowman GR**. Quantifying allosteric communication via both concerted structural changes and conformational disorder with CARDS. ***J Chem Theory Comput*** 2017;13:1509-1517.
15. Hart KM, Moeder KE, Ho CMW, Zimmerman MI, Frederick TE, **Bowman GR**. Designing small molecules to target cryptic pockets yields both positive and negative allosteric modulators. ***PLoS ONE*** 2017;12:e1078678.
16. Shen G, Cui W, Zhang H, Zhou F, Huang W, Liu Q, Yang Y, Li S, **Bowman GR**, Sadler JE, Gross ML, Li W. Warfarin traps human vitamin K epoxide reductase in an intermediate state during electron transfer. ***Nat Struct Mol Biol*** 2017;24:69-76.

17. Niu H, Fujiwara H, Martino Od, Hadwiger G, Frederick TE, Menéndez-Gutiérrez MP, Ricote M, **Bowman GR**, Welch JS. Endogenous retinoid X receptor ligands in mouse hematopoietic cells. ***Sci Signal*** 2017;10:eaan1011.
18. Halstead AM, Kapadia CD, Bolzenius J, Chu CE, Schriefer A, Wartman LD, **Bowman GR**, Arora VK. Bladder-cancer-associated mutations in RXRA activate peroxisome proliferator-activated receptors to drive urothelial proliferation. ***eLife*** 2017;6:e30862.
19. Patrick GJ, Fang L, Schaefer J, Singh S, **Bowman GR**, Wencewicz TA. Mechanistic Basis for ATP-Dependent Inhibition of Glutamine Synthetase by Tabtoxinine-β-lactam. ***Biochemistry*** 2017;57:117-135.
20. Hart KM, Ho CMW, Duta S, Gross ML, **Bowman GR**. Modeling proteins' hidden conformations to predict antibiotic resistance. ***Nat Commun*** 2016;7:12965.
21. **Bowman GR**. Accurately modeling nanosecond protein dynamics requires at least microseconds of simulation. ***J Comput Chem*** 2016;37:558-566.
22. Hart KM, Reck M, **Bowman GR**. Wencewicz TA. Tabtoxinine-β-lactam is a "stealth" β-lactam antibiotic that evades β-lactamase-mediated antibiotic resistance. ***Med Chem Comm*** 2016;7:118-127.
23. Pascolutti R, Sun X, Kao J, Maute R, Ring AM, **Bowman GR**, Kruse AC. Structure and dynamics of PD-L1 and an ultra-high-affinity PD-1 receptor mutant. ***Structure*** 2016;24:1719-1728.
24. Brosey CA, Ho C, Long WZ, Singh S, Burnett K, Hura GL, Nix JC, **Bowman GR**, Ellenberger T, Tainer JA. Defining NADH-driven allostery regulating apoptosis-inducing factor. ***Structure*** 2016;24:2067-2079.
25. Zimmerman MI, **Bowman GR**. FAST conformational searches by balancing exploration/exploitation tradeoffs. ***J Chem Theory Comput*** 2015;11:5747-5757.
26. **Bowman GR,** Bolin ER, Hart KM, Maguire BC, Marqusee S. Discovery of multiple hidden allosteric sites by combining Markov state models and experiments. ***Proc Natl Acad Sci U S A***, 2015:112;2734-2739.
27. **Bowman GR**, Geissler PL. Extensive structural heterogeneity within protein cores. ***J Phys Chem B*** 2014;118:6417-6423.
28. **Bowman GR,** Meng L, Huang X. Quantitative comparison of alternative methods for coarse-graining biological networks. ***J Chem Phys*** 2013;139:121905.
29. **Bowman GR,** Geissler PL. Equilibrium fluctuations of a single folded protein reveal a multitude of potential cryptic allosteric sites. ***Proc Natl Acad Sci U S A*** 2012;29:11681-11686.
30. **Bowman, GR**. Improved coarse-graining of Markov state models via explicit consideration of statistical uncertainty. ***J Chem Phys*** 2012;137;134111.
31. Kohlhoff KJ, Shukla D, Lawrenz M, **Bowman GR**, Konerding DE, Belov D, Altman RB, Pande VS. Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. ***Nature Chemistry,*** 2014;6:15-21.
32. Yao Y, Cui RZ, **Bowman GR**, Silva DA, Sun J, Huang X. Hierarchical Nystrom methods for constructing Markov state models for conformational dynamics. ***J Chem Phys*** 2013;138:174106.
33. Qiao Q, **Bowman GR**, Huang X. Dynamics of an intrinsically disordered protein reveal metastable conformations that potentially seed aggregation. ***J Am Chem Soc*** 2013;135:16092-16101.
34. Lin Y, **Bowman GR**, Beauchamp KA, Pande VS. Investigating how peptide length and a pathogenic mutation modify the structural ensemble of amyloid beta monomer. ***Biophys J*** 2012;102:315-324.
35. Levin AM, Bates DL, Ring AM, Krieg C, Lin JT, Su L, Moraga I, Raeber ME, **Bowman GR**, Novick P, Pande VS, Fathman CG, Boyman O, Garcia KC. Exploiting

a natural conformational switch to engineer an interleukin-2 'superkine'. ***Nature*** 2012;484:529-533.
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38. **Bowman GR**, Voelz VA, Pande VS. Atomistic folding simulations of the five-helix bundle protein $\lambda_{6\text{-}85}$. ***J Am Chem Soc*** 2011;133:664-667.
39. Silva D, **Bowman GR**, Sosa-Peinado A, Huang X. A role for both conformational selection and induced fit in ligand binding by the LAO protein. ***PLoS Comput Biol*** 2011;7:e1002054.
40. Beauchamp KA, **Bowman GR**, Lane TJ, Maibaum L, Haque IS, Pande VS. MSMBuilder2: Modeling conformational dynamics at the picosecond to millisecond scale. ***J Chem Theory Comput*** 2011;7:3412-3419.
41. Lane TJ, **Bowman GR**, Beauchamp KA, Voelz VA, Pande VS. Markov state model reveals folding and functional dynamics in ultra-long MD trajectories. ***J Am Chem Soc*** 2011;113:18413-18419.
42. Pronk S, Larsson P, Pouya I, **Bowman GR**, Haque IS, Beauchamp KA, Hess B, Pande VS, Kasson PM, Lindahl E. Copernicus: A new paradigm for parallel adaptive molecular dynamics. ***In SC '11: Proc Conf High Perf Computing, Networking, Storage and Analysis***, New York, NY, USA, 2011. ACM.
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44. **Bowman GR**, Ensign DL, Pande VS. Enhanced modeling via network theory: adaptive sampling of Markov state models. ***J Chem Theory Comput*** 2010;6:787-794.
45. Voelz VA, **Bowman GR**, Beauchamp KA, Pande VS. Molecular simulation of *ab initio* protein folding for a millisecond folder NTL9(1-39). ***J Am Chem Soc*** 2010;132:1526-1528.
46. Huang X, Yao Y, Sun J, **Bowman GR**, Guibas L, Carlsson G, Pande VS. Constructing multi-resolution Markov state models (MSMs) to elucidate RNA hairpin folding mechanisms. ***Pac Symp Biocomput*** 2010;15:228-239.
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48. **Bowman GR**, Huang X, Pande VS. Using generalized ensemble simulations and Markov state models to identify conformational states. ***Methods*** 2009;49:197-201.
49. **Bowman GR**, Pande VS. Simulated tempering yields insight into the low-resolution Rosetta scoring functions. ***Proteins*** 2009;74:777-788.
50. **Bowman GR**, Pande VS. The roles of entropy and kinetics in structure prediction. ***PLoS One*** 2009;4:e5840.
51. Huang X, **Bowman GR**, Bacallado S, Pande VS. Rapid equilibrium sampling initiated from nonequilibrium data. ***Proc Natl Acad Sci U S A*** 2009; 106:19765-19769.
52. Voelz VA, Luttmann E, **Bowman GR**, Pande VS. Probing the nanosecond dynamics of a designed three-stranded beta-sheet with a massively parallel molecular dynamics simulation. ***Int J Mol Sci*** 2009;10:1013-1030.

53. Yao Y, Sun J, Huang X, **Bowman GR**, Singh G, Lesnick M, Guibas LJ, Pande VS, Carlsson G. Topological methods for exploring low-density states in biomolecular folding pathways. ***J Chem Phys*** 2009;130:144115.
54. **Bowman GR**, Huang X, Yao Y, Sun J, Carlsson G, Guibas LJ, Pande VS. Structural insight into RNA hairpin folding intermediates. ***J Am Chem Soc*** 2008;130:9676-9678.
55. Huang X, **Bowman GR**, Pande VS. Convergence of folding free energy landscapes via application of enhanced sampling methods in a distributed computing environment. ***J Chem Phys*** 2008;128:205106.
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B. Reviews

1. Kuzmanic A, **Bowman GR**, Juarez-Jimenez J, Michel J, Gervasio FL. Investigating Cryptic Binding Sites by Molecular Dynamics Simulations. ***Acc Chem Res*** 2020;53:654-661.
2. Knoverek CR, Amarasinghe GK, **Bowman GR**. Advanced methods for accessing protein shape-shifting present new therapeutic opportunities. ***Trends Biochem Sci*** 2019;44:351-364.
3. DuBay KH, **Bowman GR,** Geissler PL. Fluctuations within folded proteins: Implications for thermodynamics and allosteric regulation. ***Acc Chem Res*** 2015;48:1098-1105.
4. Cui RZ, Silva DA, Song J, **Bowman GR**, Zhuang W, Huang X. Bridging the gap between optical spectroscopic experiments and computer simulations for fast protein folding dynamics. ***Curr Phys Chem*** 2012;2:45-58.
5. **Bowman GR**, Voelz VA, Pande VS. Taming the complexity of protein folding. ***Curr Opin Struct Biol*** 2011;21:4-11.
6. **Bowman GR**, Huang X, Pande VS. Network models for molecular kinetics and their initial applications to human health. ***Cell Research*** 2010;20:622–630.
7. Pande VS, Beauchamp KA, **Bowman GR**. Everything you wanted to know about Markov state models but were afraid to ask. ***Methods*** 2010;52:99-105.

C. Books, Monographs, Textbooks

1. Zimmerman MI, **Bowman, GR**. “How to run FAST simulations” in Computational Approaches for Studying Enzyme Mechanism Part B, Methods in Enzymology. Edited by Gregory Voth. Elsevier, 2016.
2. **Bowman GR**. “An overview and practical guide to building Markov state models” in An introduction to Markov state models and their application to long-timescale molecular simulation. Edited by **Bowman GR,** Pande VS, and Noe F. Springer Press, 2014.
3. **Bowman GR**. “Tutorial on building Markov state models with MSMBuilder and coarse-graining them with BACE” in Protein dynamics. Edited by Livesay DR. Humana Press, 2014.