Curriculum Vitae

Gregory R. Bowman

Date: 7/6/2023

Present Position

2022 - pres Louis Heyman University Professor, Departments of Biochemistry & Biophysics and Bioengineering, University of Pennsylvania
2019 - 2022 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

Teaching Title and Responsibilities

Courses
2014-2021 Chemistry and Physics of Biomolecules (course number 5357)
2014-2021 Computational Biophysics Journal Club (course number 5336)

Thesis Committees
2014-2018 Alex Holehouse
2014-2018 Kiersten Ruff
2014-2018 Tyler Harmon
2014-2018 Joshua Rackers
2014-2018 Fengbo Zhou
2014-2018 Lena Deng
2015-2018 Zhi Wang
2016-2018 Tyler Hughes
2016-2019 Sohini Sengupta
2017-2020 Matthew Matlock
2017-pres Tyson Todd
2018-2021 Patrick Judge
2019-pres Emily Wagner

2020-pres	Noah Flynn
2020-pres	Daniel Griffith
2022-pres	Helen (Claire) Woodward
2022-pres	Ryan Perez

University, School of Medicine and Hospital Appointments and Committees

2014-2020	Biochemistry Admissions Committee
2019-2021	Biochemistry Steering Committee
2021	Strategic Planning, Biomedical Research Working Group
2021-2022	Junior Faculty Search Committee
2021-2022	Cori Fellowship Steering Committee
2023-pres	Biomedical Graduate Studies Curriculum Committee
2023-pres	Biochemistry & Molecular Biophysics Program Admissions Committee

Honors and Awards

2022	Open Science Fellow, Roivant Sciences
2022	Pure Good Breakthrough Award, Pure Storage
2022	Open Science Fellow, Roivant Sciences
2021	Bio-IT World Innovation Award
2020	$4.5M hardware gift from the Pure Storage COVID-19 effort
2020	$500K hardware gift from the AMD COVID-19 HPC Fund
2020	$3M cloud computing credits from Microsoft and AWS
2020	HPCwire Reader's Choice Award for Best Use of HPC in Response to Societal Plights
2020	Featured in Microsoft CEO Satya Nadella's keynote address for the Build Developer Conference
2020	Featured in Nvidia CEO Jensen Huang's keynote address for the GTC Developer Conference
2020	Features in a 3D interactive display at Microsoft's Executive Briefing Center
2020	Featured in an ARM keynote address
2020	Featured in Financial Times https://youtu.be/bjYS0UKA4dE
2020	Featured in NHK Direct Documentary
2016-2021	Packard Fellowship for Science and Engineering
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

Trainee's Honors and Awards

2016 Center for the Science and Engineering of Living Systems Graduate Fellowship, Maxwell Zimmerman
2016-2019 Monsanto Graduate Fellowship, Maxwell Zimmerman
2017 MilliporeSigma Graduate Fellowship, Sukrit Singh
2018-2020 F-30 Ruth L. Kirschstein Individual Predoctoral NRSA for MD/PhDs, Justin Porter
2019 F-31 Ruth L. Kirschstein Predoctoral Individual NRSA, Matthew Cruz
2020 NSF MolSSI Graduate Fellowship, Michael Ward
2020 MilliporeSigma Graduate Fellowship, Catherine Knoverek
2021 MilliporeSigma Graduate Fellowship, Matthew Cruz
2020-pres Knight Alzheimer's Disease Research Postdoctoral Fellowship, Justin Miller

Editorial Responsibilities

Editor
Guest editor for PNAS
Guest editor for Frontiers in Molecular Biosciences

Reviewer
Biochimie
Biophysical Journal
Cell Reports
Chemical Physics Letters
Chemical Reviews
Current Opinions in Structural Biology
eLife
Entropy
Journal of Chemical Education
Journal of Chemical Information and Modeling
Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Computational Chemistry
Journal of Lipid Research
Journal of Molecular Biology
Journal of Molecular Graphics and Modeling
Journal of Physical Chemistry B
Journal of Physical Chemistry Letters
Journal of Structural Biology
Journal of the American Chemical Society

Nature
Nature Communications
Physical Review Letters
Physical Review X
PLoS Computational Biology
PLoS ONE
Proceeding of the National Academy of Sciences
Proteins: structure, function and bioinformatics
Scientific Reports
WIRES Computational Molecular Science

Community Service Contributions

Community Service

2014-2018	Organize Molecular Kinetics in Drug Discovery Workshop
2018-pres	Director of the Folding@home distributed computing project
2014-pres	Outreach to the visually impaired through organizations like the Foundation Fighting Blindness
2020-pres	Organize a monthly video conference for visually-impaired people in STEM that includes graduate students, postdocs, faculty, and STEM professionals from around the globe

Professional Societies

2008-pres	Biophysical Society
2008-pres	American Chemical Society
2021-pres	Protein Society

Major Invited Professorships and Lectureships

2024 Protein Folding Dynamics GRC, Galveston, TX
2024 Markov State Modeling of Conformational Dynamics ACS Symposium, New Orleans, LA
2024 Machine Learning Meets Statistical Mechanics CECAM, Sorrento, Italy
2023 New Concepts in Drug Discovery and Engineering AACR Plenary, Orlando, FL
2023 Computer Aided Drug Design GRC, Mount Snow, VT
2023 Molecular Machine Learning Keynote at Mila, Montreal, Canada
2023 Graham Lecture, UVA, VA
2023 Rare Events Workshop at Brin MRC, UMD, MD
2023 Integrative Modeling Seminar Series
2023 Drug Discovery Seminar, Incyte Biopharmaceutical
2023 Machine Learning Seminar, IQVIA
2022 Biophysics at the Dawn of Exascale Computing, Hamburg, Germany
2022 Machine Learning Meets Statistical Mechanics CECAM, Sorrento, Italy
2022 Council for Scientific Society Presidents, Washington DC
2022 Machine Learning and Informatics for Chemistry & Materials, Telluride, CO
2022 Gibbs Conference on Biological Thermodynamics, , Carbondale, IL
2022 Office of Data Science Strategy Seminar, NIH

2022 Biophysics Seminar, UCSF
2022 Physiology Seminar, Loyola University
2022 Biophysics Seminar, Arizona State University
2022 Computational Biology Seminar, University of Kansas
2022 Drug Discovery Seminar, Nested Therapeutics
2022 Drug Discovery Seminar, Roivant Sciences
2022 Drug Discovery Seminar, Third Rock Ventures
2021 Computational Chemistry in Addressing COVID-19, ACS Sprint Meeting
2021 Computational Chemistry of COVID-19, ACS Fall Meeting
2021 Computer-aided Drug Discovery GRC
2021 Under-represented Groups in Computational Chemistry
2021 Office of Data Science Strategy Seminar, NIH
2021 Biochemistry Seminar, Yale
2021 Biological Engineering Seminar, U Penn
2021 Chemistry Seminar, MIT
2021 Biochemistry Seminar, UW Madison
2021 CogX Festival
2021 AI Salon, Stanford, CA
2021 HPC-AI Conference, Stanford, CA
2021 Biophysics Seminar, UIUC Beckman Institute, IL
2021 Weighted Ensembles Workshop
2021 RARE Simulation Algorithm Meeting, India
2021 NSF Lightning Talk
2021 AMD HPC Forum
2021 Atomwise Seminar
2021 Swiss HPC-AI Advisory Council
2021 Cambridge Healthcare Institute
2021 Folding@home Symposium
2020 Pharmaceutical Biophysics Symposium, Biophysical Society
2020 Chemistry Seminar, UIUC, IL
2020 SAGIM drug design community, San Diego
2020 Pharmacology Seminar, Case Western Reserve University, OH
2020 Financial Times Interview
2020 NHK Direct Documentary on Folding@home
2020 JEDI SARS-CoV-2 Drug Discovery Symposium
2020 CERN
2020 IEEE InTech
2020 ARM DevSummit
2020 VMworld Developer Summit
2020 Dell HPC Working Group
2020 Avast SARS-CoV-2 Seminar
2020 a16z (Andreessen Horowitz) Podcast
2020 Microsoft Build Developer Summit
2020 Oracle Kickin it With Karan Video Interview
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
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

Consulting Relationships and Board Memberships

Trainee/Mentee/Sponsorship Record:

Current advisees

Postdoctoral Fellows

2021-pres Justin Miller
2021-pres Louis Smith
2022-pres Prajna Mishra
2023-pres Bhupendra Dandekar

Graduate Students

2019-pres Upasana Mallimadugula, Biochemistry, Biophysics, and Structural Biology
2022-pres Devin Kelly, Biochemistry & Molecular Biophysics
2023-pres Shahlo Solieva, Biochemistry & Molecular Biophysics
2023-pres Mark Bray, Biochemistry & Molecular Biophysics

Undergraduate students
2023-pres Anthony Trent
2023-pres Anne Gumina

Past advisees
Staff
2014-2017 Katherine Hart, Research Assistant Professor
Next an Assistant Professor at Williams College
2015-2017 Carrie Sibbald, Technician
Next a medical student at Washington University
2017-2018 Katelyn Moeder
Next a medical student at Oklahoma State University
2020-2021 Catherine Kuhn
Now a graduate student at UCSF
2021-2022 Jonathan Borowsky
Now a graduate student at UCSF

Postdoctoral Fellows
2014-2016 Xianqiang (Leos) Sun, Postdoctoral Fellow
Next a scientist at the pharmaceutical company WuXi AppTec
2016-2019 Thomas Frederick
Next a staff scientist at AbvVie
2018-2022 Neha Vithani
Next a Scinetist at OpenEye
2019-2021 Maxwell Zimmerman
Next a scientist at Generate
2021-2022 Soumendranath Bhakat
Next a scientist at Redesign

Graduate Students
2015-2019 Maxwell Zimmerman, Computational and Molecular Biophysics
Next a postdoc in my group
2016-2020 Justin Porter, MSTP, Computational and Systems Biology
Next finishing medical school at Washington University
2015-2020 Sukrit Singh, Computational and Molecular Biophysics
Next a postdoc at Memorial Sloan Kettering
2016-2021 Catherine Knoverek, Computational and Molecular Biophysics
Next a scientist at Thermo
2018-2023 Matthew Cruz, Biochemistry, Biophysics, and Structural Biology
Next a postdoc at Merck

2019-2022 Michael Ward, Computational and Systems Biology
Next a scientist at Generate
2019-2023 Artur Meller, Computational and Systems Biology
Next finishing medical school at Washington University

Undergraduates
2014-2017 Katelyn Moeder
2016-2017 Katelyn Miyasaki
2018 Antony Sagayaraj
2017-2020 Shreya Raavicharla
2018-2020 Emily Wood
2019-2020 Catherine Kuhn
2019-2021 Jonathan Borowsky
2020-2022 Rishi Samarth
2022-2023 Ayan Bhattacharjee

Bibliography:

A. Original Articles

1. Meller A, Lotthammer JM, Smith LG, Novak B, Lee LA, Kuhn CC, Greenberg L, Leinwand LA, Greenberg MJ, **Bowman GR**. Drug specificity and affinity are encoded in the probability of cryptic pocket opening in myosin motor domains. ***Elife*** 2023;12:e83602.
2. Meller A, Ward M, Borowsky J, Lotthammer JM, Kshirsagar M, Oviedo F, Ferres JL, **Bowman GR**. Predicting locations of cryptic pockets from single protein structures using the PocketMiner graph neural network***. Nature Communications*** 2022;14:1177.
3. Meller A, Bhakat S, Solieva S, **Bowman GR**. Accelerating Cryptic Pocket Discovery Using AlphaFold***. J Chem Theory Comput***. 2023 in press.
4. Stuchell-Brereton MD, Zimmerman MI, Miller JJ, Mallimadugula UL, Incicco JJ, Roy D, Smith LG, Cubuk J, Baban B, DeKoster GT, Frieden C, **Bowman GR**, Soranno A. Apolipoprotein E4 has extensive conformational heterogeneity in lipid-free and lipid-bound forms. ***Proceedings of the National Academy of Sciences*** 2023;120:e2215371120.
5. Meller A, De Oliveira S, Davtyan A, Abramyan T, **Bowman GR**, van den Bedem H. Discovery of a cryptic pocket in the AI-predicted structure of PPM1D phosphatase explains the binding site and potency of its allosteric inhibitors. ***Front Mol Biosci***. 2023;10:1171143.
6. Lee LA, Barrick SK, Meller A, Walklate J, Lotthammer JM, Tay JW, Stump WT, **Bowman GR**, Geeves MA, Greenberg MJ, Leinwand LA. Functional divergence of the sarcomeric myosin, MYH7b, supports species-specific biological roles. ***Journal of Biological Chemistry*** 2023;299:102657.
7. Tamadonfar KO, Venanzio GD, Pinkner JS, Dodson KW, Kalas V, Zimmerman MI, Villicana JB, **Bowman GR**, Feldman MF, Hultgren SJ. Structure–function correlates of fibrinogen binding by Acinetobacter adhesins critical in catheter-

associated urinary tract infections. ***Proceedings of the National Academy of Sciences*** 2023;120:e2212694120.

8. Cruz MA, Frederick TE, Mallimadugula UL, Singh S, Vithani N, Zimmerman MI, Porter JR, Moeder KE, Amarasinghe GK, **Bowman GR**. A cryptic pocket in Ebola VP35 allosterically controls RNA binding. ***Nature Communications*** 2022;13:2269.
9. Meller A, Bhakat S, Solieva S, **Bowman GR**. Accelerating cryptic pocket discovery using AlphaFold. ***bioRxiv*** 2022:2022.11. 23.517577.
10. Huang Z, Liu H, Nix J, Xu R, Knoverek CR, **Bowman GR**, Amarasinghe GK, Sibley LD. The intrinsically disordered protein TgIST from Toxoplasma gondii inhibits STAT1 signaling by blocking cofactor recruitment. ***Nature Communications*** 2022;13:1-15.
11. Jansen J, Reimer KC, Nagai JS, Varghese FS, Overheul GJ, Beer Md, Roverts R, Daviran D, Fermin LA, Willemsen B, Beukenboom M, Djudjaj S, Stillfried Sv, Eijk LEv, Mastik M, Bulthuis M, Dunnen Wd, Goor Hv, Hillebrands J, Triana SH, Alexandrov T, Timm M, Berge BTvd, Broek Mvd, Nlandu Q, Heijnert J, Bindels EM, Hoogenboezem RM, Mooren F, Kuppe C, Miesen P, Grünberg K, Ijzermans T, Steenbergen EJ, Czogalla J, Schreuder MF, Sommerdijk N, Akiva A, Boor P, Puelles VG, Floege J, Huber TB, Achdout H, Aimon A, Bar-David E, Barr H, Ben-Shmuel A, Bennett J, Boby ML, Borden B, **Bowman GR**, Brun J, BVNBS S, Calmiano M, Carbery A, Cattermole E, Chernychenko E, Choder JD, Clyde A, Coffland JE, Cohen G, Cole J, Contini A, Cox L, Cvitkovic M, Dias A, Donckers K, Dotson DL, Douangamath A, Duberstein S, Dudgeon T, Dunnett L, Eastman PK, Erez N, Eyermann CJ, Fairhead M, Fate G, Fearon D, Federov O, Ferla M, Fernandes RS, Ferrins L, Foster R, Foster H, Gabizon R, Garcia-Sastre A, Gawriljuk VO, Gehrtz P, Gileadi C, Giroud C, Glass WG, Glen R, Godoy AS, Gorichko M, Gorrie-Stone T, Griffen EJ, Hart SH, Heer J, Henry M, Hill M, Horrell S, Hurley MF, Israely T, Jajack A, Jnoff E, Jochmans D, John T, Jonghe SD, Kantsadi AL, Kenny PW, Kiappes J, Koekemoer L, Kovar B, Krojer T, Lee AA, Lefker BA, Levy H, London N, Lukacik P, Macdonald HB, Maclean B, Malla TR, Matviiuk T, McCorkindale W, McGovern BL, Melamed S, Michurin O, Mikolajek H, Milne BF, Morris A, Morris GM, Morwitzer MJ, Moustakas D, Nakamura AM, Neto JB, Neyts J, Nguyen L, Noske GD, Oleinikovas V, Oliva G, Owen D, Psenak V, Pai R, Pan J, Paran N, Perry B, Pingle M, Pinjari J, Politi B, Powell A. SARS-CoV-2 infects the human kidney and drives fibrosis in kidney organoids***.*** ***Cell Stem Cell*** 2022;29:217-231. e8.
12. Knapp BD, Ward MD, ***Bowman GR***, Shi H, Huang KC. Multiple conserved states characterize the twist landscape of the bacterial actin homolog MreB. ***Computational and Structural Biotechnology Journal*** 2022;20:5838-5846.
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14. Eguchi RR, Choe CA, Parekh U, Khalek IS, Ward MD, Vithani N, **Bowman GR**, Jardine JG, Huang P. Deep Generative Design of Epitope-Specific Binding

Proteins by Latent Conformation Optimization. ***bioRxiv*** 2022:2022.12.22.521698.

15. Zimmerman MI, Porter JR, Ward MD, Singh S, Vithani N, Meller A, Mallimadugula UL, Kuhn CE, Borowsky JH, Wiewiora RP, Hurley MF, Harbison AM, Fogarty CA, Coffland JE, Fadda E, Voelz VA, Chodera JD, **Bowman GR**. SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. ***Nature Chemistry*** 2021;13:651-659.
16. Ward MD, Zimmerman MI, Meller A, Chung M, Swamidass S, **Bowman GR**. Deep learning the structural determinants of protein biochemical properties by comparing structural ensembles with DiffNets. ***Nature Communications*** 2021;12:1-12.
17. Knoverek CR, Mallimadugula UL, Singh S, Rennella E, Frederick TE, Yuwen T, Raavicharla S, Kay LE, ***Bowman GR***. Opening of a cryptic pocket in β-lactamase increases penicillinase activity. ***Proceedings of the National Academy of Sciences*** 2021;118:e2106473118.
18. Vithani N, Ward MD, Zimmerman MI, Novak B, Borowsky JH, Singh S, **Bowman GR**. SARS-CoV-2 Nsp16 activation mechanism and a cryptic pocket with pan-coronavirus antiviral potential. ***Biophysical Journal*** 2021;120:2880-2889.
19. Cubuk J, Alston JJ, Incicco JJ, Singh S, Stuchell-Brereton MD, Ward MD, Zimmerman MI, Vithani N, Griffith D, Wagoner JA, ***Bowman GR***, Hall KB, Soranno A, Holehouse AS. The SARS-CoV-2 nucleocapsid protein is dynamic, disordered, and phase separates with RNA. ***Nature Communications*** 2021;12:1-17.
20. Malik M, Ward MD, Fang Y, Porter JR, Zimmerman MI, Koelblen T, Roh M, Frolova AI, Burris TP, ***Bowman GR***, Imoukhuede PI, England SK. Naturally Occurring Genetic Variants in the Oxytocin Receptor Alter Receptor Signaling Profiles. ***ACS Pharmacology & Translational Science*** 2021;4:1543-1555.
21. Achdout H, Aimon A, Bar-David E, Barr H, Ben-Shmuel A, Bennett J, Boby ML, Borden B, **Bowman GR**, Brun J, BVNBS S, Calmiano M, Carbery A, Cattermole E, Chernyshenko E, Chodera JD, Clyde A, Coffland JE, Cohen G, Cole J, Contini A, Cox L, Cvitkovic M, Dias A, Donckers K, Dotson DL, Douangamath A, Duberstein S, Dudgeon T, Dunnett L, Eastman PK, Erez N, Eyermann CJ, Fairhead M, Fate G, Fearon D, Fedorov O, Ferla M, Fernandes RS, Ferrins L, Foster R, Foster H, Gabizon R, Garcia-Sastre A, Gawriljuk VO, Gehrtz P, Gileadi C, Giroud C, Glass WG, Glen R, Glinert I, Godoy AS, Gorichko M, Gorrie-Stone T, Griffen EJ, Hart SH, Heer J, Henry M, Hill M, Horrell S, Hurley MF, Israely T, Jajack A, Jnoff E, Jochmans D, John T, Jonghe SD, Kantsadi AL, Kenny PW, Kiappes J, Koekemoer L, Kovar B, Krojer T, Lefker BA, Levy H, London N, Lukacik P, Macdonald HB, MacLean B, Malla TR, Matviiuk T, McCorkindale W, McGovern BL, Melamed S, Michurin O, Mikolajek H, Milne BF, Morris A, Morris GM, Morwitzer MJ, Moustakas D, Nakamura AM, Neto JB, Neyts J, Nguyen L, Noske GD, Oleinikovas V, Oliva G, Overheul GJ, Owen D, Psenak V, Pai R, Pan J, Paran N, Perry B, Pingle M, Pinjari J, Politi B, Powell A, Puni R, Rangel VL, Reddi RN, Reid SP, Resnick E, Ripka EG, Robinson MC, Robinson RP, Rodriguez-Guerra J, Rosales R, Rufa D, Schofield C, Shafeev M, Shaikh A, Shi J, Shurrush K, Singh S, Sittner A, Skyner R, Smalley A, Smilova MD, Solmesky

LJ, Spencer J, Strain-Damerell C, Swamy V, Tamir H, Tennant R, Thompson W, Thompson A, Tomasio S, Tumber A, Vakonakis I, Rij RPv, Vangeel L, Varghese FS, Vaschetto M, Vitner EB, Voelz V, Volkamer A, Delft Fv, Delft Av. Open Science Discovery of Oral Non-Covalent SARS-CoV-2 Main Protease Inhibitor Therapeutics. ***bioRxiv*** 2021:2020.10. 29.339317.

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23. Porter JR, Meller A, Zimmerman MI, Greenberg MJ, **Bowman GR**. Conformational distributions of isolated myosin motor domains encode their mechanochemical properties. ***eLife*** 2020;9:e55132.
24. 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.
25. 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.
26. Brown CA, Hu L, Sun Z, Patel MP, Singh S, Porter PR, Sankaran B, Prasad BVV, **Bowman GR**, Palzkill T. Antagonism between substitutions in β-lactamase explains a path not taken in the evolution of bacterial drug resistance. ***J Biol Chem***. 2020;295:7376-7390.
27. Riehl JR, Zimmerman MI, Singh MF, Bowman GR, Ching S. Computing and optimizing over all fixed-points of discrete systems on large networks. ***Journal of the Royal Society Interface*** 2020;17:20200126.
28. 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.
29. Porter JR, Zimmerman MI, **Bowman GR**. Enspara: Modeling molecular ensembles with scalable data structures and parallel computing. ***J Chem Phys*** 2019;150:044108.
30. 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.
31. 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.
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33. 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.
34. 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.
35. 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.
36. 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.
37. 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.
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