Gabriel J. Rocklin, Ph.D.

email grocklin@gmail.com
web http://gabrielrocklin.me
tel (408) 835-5235
mailing University of Washington
Molecular Engineering and Sciences
4000 15th Ave NE, Box 351655
Seattle, WA 98195

Electronic CV with hyperlinks available at http://gabrielrocklin.me

Education

2013 - **Senior Fellow, Department of Biochemistry, University of Washington**
Advisor: David Baker

2007 - 2013 **PH.D. in Biophysics, University of California, San Francisco**
Advisors: Brian Shoichet, Ken Dill
Thesis: Predicting charged protein-ligand binding affinities using free energy calculations

2003 - 2007 **B.A. in Biology-Chemistry & History, Claremont McKenna College**, *summa cum laude*
Undergraduate research with Emily Wiley (*Tetrahymena* epigenetics)

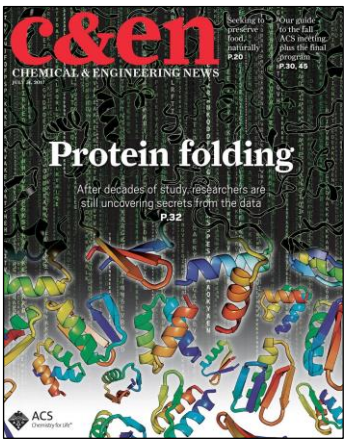
Fellowships and Awards

2014 - 2017 Merck Postdoctoral Fellow of the Life Sciences Research Foundation
2009 - 2012 National Defense Science and Engineering Graduate Fellowship
2008 - 2013 National Science Foundation Graduate Research Fellowship
2008 1st Place, U.C. Berkeley Science, Technology & Engineering Policy White Paper Competition
"Promoting Pharmaceutical Research under National Health Care Reform" (*with Jacob Heller*)
2007 Top Graduating Senior in Science, Claremont McKenna College

Publications

10 total | 6 first-authored | 2 corresponding-authored
Google scholar statistics: http://goo.gl/fHzUl

10 DOI Chevalier A*, Silva D-A*, **Rocklin GJ***, Hicks DR, Vergara R, Murapa P, Bernard S, Zhang L, Lam K-H, Yao G, Bahl CD, Miyashita S-I, Goreshnik I, Fuller JT, Koday MT, Jenkins C, Colvin T, Carter L, Bohn A, Bryan CM, Fernandez-Velasco DA, Stewart L, Dong M, Huang X, Jin R, Wilson IA, Fuller DH, Baker D. Massively parallel de novo protein design for targeted therapeutics. *Nature* 550, 74-79 (2017) **contributed equally*
Research highlights: *Cell*, *Biochemistry*
News coverage: *The New York Times*, *Chemical & Engineering News*, *In the Pipeline*



9 DOI **Rocklin GJ**, Chidyausiku TM, Goreshnik I, Ford A, Houliston S, Lemak A, Carter L, Ravichandran R, Mulligan VK, Chevalier A, Arrowsmith CH, Baker D. Global analysis of protein folding using massively parallel design, synthesis, and testing. *Science* 357, 168-75 (2017)
Perspective by Woolfson et al. | Recommendations on Faculty of 1000 Prime
Research highlights: *Nature Chemical Biology*, *Nature Methods*
News coverage: *Chemical & Engineering News* (with my cover art), *Chemistry World*, *ACCN (Canadian Chemical News)*, *Genetic Engineering & Biotechnology News*, *The Scientist*

8 DOI Bhardwaj G*, Mulligan VK*, Bahl CD*, Gilmore JM, Harvey PJ, Cheneval O, Buchko GW, Pulavarta SVSRK, Kass Q, Eletsky A, Huang P-S, Johnsen WA, Greisen PJ, **Rocklin GJ**, Song Y, Linsky TW, Watkins A, Rettie SA, Xu X, Carter LP, Bonneau R, Olson JM, Coutsias E, Correnti CE, Szyperski T, Craik DJ, Baker D. Accurate de novo design of hyperstable constrained peptides. *Nature* 538, 329-35 (2016)

7 DOI **Rocklin GJ**, Mobley DL, Dill KA, Hünenberger PE. Calculating the binding free energies of charged species based on explicit-solvent simulations employing lattice-sum methods: An accurate correction scheme for electrostatic finite-size effects. *J Chem Phys* 139, 184103 (2013)
Recommendation on Faculty of 1000 Prime | Featured Cover Article

6 DOI **Rocklin GJ***, Boyce SE*, Fischer M*, Fish I, Mobley DL, Shoichet BK, Dill KA. Blind prediction of charged ligand binding affinities in a model binding site. *J Mol Biol* 425, 4569-83 (2013)
Recommendation on Faculty of 1000 Prime

5 DOI **Rocklin GJ†**, Mobley DL, Dill KA. Calculating the Sensitivity and Robustness of Binding Free Energy Calculations to Force Field Parameters. *J Chem Theory Comput* 9:7, 3072-83 (2013)

4 DOI **Rocklin GJ†**, Mobley DL, Dill KA. Separated Topologies – a Method for Relative Binding Free Energy Calculations using Orientational Restraints. *J Chem Phys* 138, 085104 (2013)

3 DOI Boyce SE*, Mobley DL*, **Rocklin GJ**, Graves AP, Dill KA, Shoichet BK. Predicting ligand binding affinity with alchemical free energy methods in a polar model binding site. *J Mol Biol* 394, 747-63 (2009)

2 DOI Teotico DG*, Babaoglu K*, **Rocklin GJ**, Ferreira RS, Giannetti AM, Shoichet BK. Docking for fragment inhibitors of AmpC beta-lactamase. *Proc Natl Acad Sci U S A* 106, 7455-60 (2009)

1 DOI DerMardirossian C, **Rocklin G**, Seo JY, Bokoch GM. Phosphorylation of RhoGDI by Src Regulates RhoGTPase Binding and Cytosol-Membrane Cycling. *Mol Biol Cell* 17, 4760-8 (2006)

* *denotes equal contribution*
† *denotes corresponding authorship*

Invited Talks

2018 PDF RosettaCON 2018, Leavenworth WA
The structural basis for protein energy landscapes in a *de novo* designed proteome

2018 Genentech. Invited seminar, South San Francisco CA
Massively parallel design and testing of new protein folds and targeted inhibitors

2018 PDF Chemistry and Biology of Peptides Gordon Research Conference 2018, Ventura CA
Massively parallel design and testing of new protein folds and targeted inhibitors

2018 Just. biotherapeutics for all. Invited seminar, Seattle WA
Massively parallel design and testing of new protein folds and targeted inhibitors

2018 PDF PepTalk 2018, Keynote Presentation for Higher-Throughput Protein Production & Characterization
Massively parallel design and testing of new protein folds and targeted inhibitors

2017 Biogen. Invited seminar, Cambridge MA
Massively parallel design and testing of new protein folds and targeted inhibitors

2017 PDF Council of Scientific Society Presidents Winter Meeting, "Frontiers of Science", Washington D.C.
Massively parallel design of new protein folds and targeted inhibitors

2017 PDF Rising Stars Symposium, University of Utah Biochemistry Department
Global analysis of protein folding using massively parallel design, synthesis, and testing

2015 PDF RosettaCON 2015, Leavenworth WA
High throughput protein design at the edge of folding (Best Talk Award)

2014 Laufer Center for Physical and Quantitative Biology, Stony Brook University
Designing protein structures de novo the Rosetta way

2014 PDF Free Energy Methods in Drug Design Workshop, Vertex Pharmaceuticals
Analytical corrections for charged compound binding affinities computed from periodic simulations

2013 PPT 5-College Chemistry Seminar, Claremont Colleges
Molecular dynamics simulations for drug discovery

2012 PPT Free Energy Methods in Drug Design Workshop, Vertex Pharmaceuticals
Testing alchemical free energy calculations in a charged model site

Poster Presentations

2017 PDF Proteins Gordon Research Conference, Holderness NH
Global analysis of protein folding using massively parallel design, synthesis, and testing

2017 PDF Biophysical Society Annual Meeting, New Orleans LA
Global analysis of protein folding using massively parallel design, synthesis, and testing

2015 PDF Proteins Gordon Research Conference, Holderness NH
De novo protein design of AMA1 inhibitors for malaria

2012 PDF OpenEye CUP XII, Santa Fe, NM
Predicting Absolute Protein-Ligand Binding Affinities of Charged Molecules using Free Energy Calculations

2010 PDF Free Energy Methods in Drug Design Workshop, Vertex Pharmaceuticals
Predicting Absolute Protein-Ligand Binding Affinities of Charged Molecules using Free Energy Calculations

Grants Written

2011 340,556 Teragrid Compute Hours (awarded to Brian Shoichet)
"Can molecular dynamics simulations predict the binding affinities of compounds in a realistic fragment screen?"

2010 706,000 Teragrid Compute Hours (awarded to Brian Shoichet)
"Can MD simulations predict the binding affinities of charged ligands to a model protein binding site?"

Academic Service

2017 Small group discussion leader on community diversity and inclusion, RosettaCON

2015 – now Code of Conduct Committee, RosettaCON

2013 - Reviewer - *Journal of Chemical Physics*, *Journal of Chemical Theory and Computation*

Teaching Experience

2017 Instructor, BIS 285 B "An Ounce of Prevention: Vaccines in Science and Society" (3 credit seminar)
Winter 2017 term, University of Washington (Bothell campus)
Co-designed and co-taught undergraduate seminar course with two other postdocs, with faculty mentorship provided through the University of Washington Science Teaching Experience for Postdocs Fellowship

2017 Keynote Lecture, Washington Jr. Science & Humanities Symposium
Computational protein design on a massive scale: Big molecules meet big data

2014 Guest Lecture, Lynbrook High School Science Club
Computational protein design

2012 Guest Lecture, Lynbrook High School Science Club
Predicting protein-ligand binding using computer simulations

2011 Career fair presentation, Homestead High School Career Fair
Careers in Scientific Research

2008-2011 Teaching Assistant, UCSF Biophysics Bootcamp
Led small group discussions. Lectured on computational biophysical methods. Assisted with Python classes.

2010 Guest Lecture, U.C. Berkeley E39B Introduction to Computational Engineering
Computational Biology

2009 Teaching Assistant, UCSF NSF Graduate Research Fellowship Program Application Workshop
Guided first-year graduate students through fellowship applications; edited and revised proposals

2009 Teaching Assistant, UCSF BP204B Macromolecular Interactions
Assisted first-year graduate students in methods and theory of macromolecules and preparing a research proposal

2003-2005 Volunteer Debate Coach, Alta Loma High School
Taught public speaking and formal argumentation strategy. Travelled with students to local and state tournaments.

Student Mentoring

2016 – now	Tamuka Chidyausiku	Baker Lab Ph.D. research (coauthor)
2015 – now	Ta-Yi Yu	Baker Lab Ph.D. rotation and ongoing research
2015	Chris Woods	Baker Lab Ph.D. rotation

References

David Baker, Ph.D.
Professor
Department of Biochemistry
University of Washington
(206) 543-1295
dabaker@u.washington.edu

Brian K. Shoichet, Ph.D.
Professor
Department of Pharmaceutical Chemistry
University of California, San Francisco
(415) 514-4253
bshoichet@gmail.com

Ken A. Dill, Ph.D.
Professor
Laufer Center for Physical and Quantitative Biology
Stony Brook University
(613) 632-5400
dill@laufercenter.org