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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

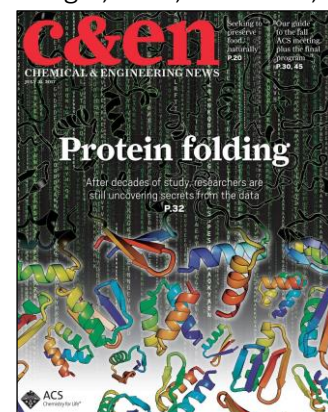
- 2014 - 2017 Merck Postdoctoral Fellow of the Life Sciences Research Foundation
- 2009 - 2012 National Defense Science and Engineering Graduate Fellowship
- 2008 - 2013 National Science Foundation Graduate Research Fellowship
- 2008 1st Place, U.C. Berkeley Science, Technology & Engineering Policy White 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/fHzUI>

- 10 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*, in press, 2017 **contributed equally*
- 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*



- 8 DOI Bhardwaj G*, Mulligan VK*, Bahl CD*, Gilmore JM, Harvey PJ, Cheneval O, Buchko GW, Pulavarta SVSRK, Kass Q, Eletsy 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, Coutsiar 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

- 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

Upcoming:

- 2017 Rising Stars Symposium, University of Utah Biochemistry Department
- 2017 Council of Scientific Society Presidents Winter Meeting, “Frontiers of Science”, Washington D.C.
- 2018 Keynote Presentation, Higher-Throughput Protein Production & Characterization, PepTalk 2018

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 K. 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 K. 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

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.
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Brian K. Shoichet, Ph.D.
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Ken A. Dill, Ph.D.
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