Gabriel J. Rocklin, Ph.D.

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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/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*
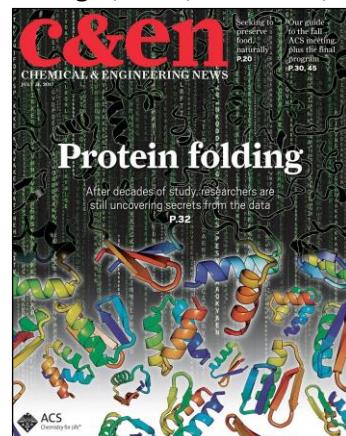
8   DOI   Bhardwaj G*, Mulligan VK*, Bahl CD*, Gilmore JM, Harvey PJ, Cheneval O, Buchko GW, Pulavarta SVSRK, Kass Q, Eletsky A, Huang P-S, Johnsen WA, Greisen PJ, **Rocklin GJ**, Song Y, Linsky TW, Watkins A, Rettie SA, Xu X, Carter LP, Bonneau R, Olson JM, Coutsias E, Correnti CE, Szyperski T, Craik 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   Chemistry and Biology of Peptides Gordon Research Conference 2018, Ventura CA
      Massively parallel design and testing of new protein folds and targeted inhibitors

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

2017   Biogen, Inc. 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

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