

Kimberly A. Reynolds

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Education

Ph.D in Biophysics University of California, Berkeley. Advisor: Dr. Tracy M. Handel	Dec. 2006
B.A. in Biochemistry Rice University, Houston, TX.	2001

Research and Professional Experience

Assistant Professor Green Center for Systems Biology and Dept. of Biophysics UT Southwestern Medical Center, Dallas, TX	2014-present
Postdoctoral Researcher – <i>Advisor: Dr. Rama Ranganathan</i> Green Center for Systems Biology, UT Southwestern Medical Center, Dallas, TX	2008-2014
Postdoctoral Researcher – <i>Advisors: Dr. Ruben Abagyan and Dr. Ed Roberts</i> Department of Molecular Biology, The Scripps Research Institute, La Jolla	2007-2008
Adjunct Professor – <i>mentored teaching fellowship</i> Department of Chemistry, University of San Diego, CA	Fall 2007

Awards and Fellowships

Biophysical Society – Biopolymers in vivo subgroup Young Faculty Award	2022
Outstanding Graduate Educator – UT Southwestern Academy of Teachers	2020
National Science Foundation CAREER award	2020
Scialog Fellow, Molecules Come to Life Program	2016
Data Driven Discovery Investigator, Gordon and Betty Moore Foundation	2014
Alfred Gilman award for excellence in postdoctoral research, UTSW	2011
Scripps/USD JUST program mentored undergraduate teaching internship	2007
National Science Foundation Graduate Research Fellow	2003-2006
Achievement Rewards for College Scholars (ARCS) Graduate Fellow	2001-2003

Publications

1. R.M. Otto, A. Turska-Nowak, P.M. Brown, **K.A. Reynolds** (2022). A continuous epistasis model for predicting growth rate given combinatorial variation in gene expression and environment. BioRxiv. <https://doi.org/10.1101/2022.08.19.504444>

2. J. McCormick, M.A.X. Russo, S. Thompson, A. Blevins, **K.A. Reynolds** (2021). Structurally distributed surface sites tune allosteric regulation. *Elife* (10):e68346. <https://doi.org/10.7554/elife.68346>
3. **K.A. Reynolds**, E. Rosa-Molinar, R.E. Ward, H. Zhang, B.R. Urbanowicz, A.M. Settles (2021). Accelerating biological insight for understudied genes. *Integr Comp Biol* (icab029). <https://doi.org/10.1093/icb/icab029>
4. A.D. Mathis, R.M. Otto, **K.A. Reynolds** (2021). A simplified strategy for titrating gene expression reveals new relationships between genotype, environment, and bacterial growth. *Nucleic Acids Research* (49):e6. <https://doi.org/10.1093/nar/gkaa1073>
5. S. Thompson, Y. Zhang, C. Ingle, **K.A. Reynolds**, and T. Kortemme (2020). Altered expression of a quality control protease in *E. coli* reshapes the *in vivo* mutational landscape of a model enzyme. *Elife* (9):e53476. <https://doi.org/10.7554/eLife.53476>
6. J.W. McCormick, D. Pincus, O. Resnekov, and **K.A. Reynolds** (2019). Strategies for engineering and rewiring kinase regulation. *Trends Biochem Sci* (19):30234. <https://doi.org/10.1016/j.tibs.2019.11.005>
7. A.F.Schober, A.D. Mathis, C.Ingle, J.O. Park, L. Chen, J.D. Rabinowitz, I. Junier, O. Rivoire, and **K.A. Reynolds** (2019). A two-enzyme adaptive unit within bacterial folate metabolism. *Cell Reports* (27):3359. <https://doi.org/10.1016/j.celrep.2019.05.030>
8. Y.T. Tamer, I.K. Gaszek, H. Abdizadeh, T. Batur, **K. Reynolds**, A.R. Atilgan, C. Atilgan, E. Toprak (2019). High-order epistasis in catalytic power of dihydrofolate reductase gives rise to a rugged fitness landscape in the presence of trimethoprim selection. *Molecular Biology and Evolution* (36):1533. <https://doi.org/10.1093/molbev/msz086>
9. D. Pincus, J. Pandey, Z.A. Feder, P. Creixell, O. Resnekov, and **K.A. Reynolds** (2018). Engineering allosteric regulation in protein kinases. *Science Signaling* (11):555. <https://doi.org/10.1126/scisignal.aar3250>
10. C. Rosensweig, **K.A. Reynolds**, P. Gao, Y. Shan, R. Ranganathan, J.S. Takahashi, C.B Green (2018). An evolutionary hotspot defines functional differences between CRYPTOCHROMES. *Nature Communications* (9):1138. <http://dx.doi.org/10.1038/s41467-018-03503-6>
11. C. Narayanan, D. Gagné, **K.A. Reynolds**, N. Doucet (2017). Conserved amino acid networks modulate discrete functional properties in an enzyme superfamily. *Scientific Reports* (7):3207. <http://dx.doi.org/10.1038/s41598-017-03298-4>
12. D. Pincus, O. Resnekov, **K.A. Reynolds** (2017). An evolution-based strategy for engineering allosteric regulation. *Physical Biology* (14): 025002. <http://dx.doi.org/10.1088/1478-3975/aa64a4>
13. O. Rivoire, **K.A. Reynolds**, R. Ranganathan (2016). Evolution-based functional decomposition of proteins. *PLoS Comp Biol* (12): e1004817. <http://dx.doi.org/10.1371/journal.pcbi.1004817>
Associated software: <http://reynoldsk.github.io/pySCA/>

14. **K.A. Reynolds** (2015). A new test of computational protein design: predicting posttranslational modification specificity for the enzyme SMYD2. *Structure* (23):11. <http://dx.doi.org/10.1016/j.str.2014.12.004>
15. **K.A. Reynolds** (2014). Finding a common path: predicting gene function using inferred evolutionary trees. *Developmental Cell* (30):4. <http://dx.doi.org/10.1016/j.devcel.2014.06.029>
16. **K.A. Reynolds**, W. P. Russ, M. Socolich, R. Ranganathan (2013). Evolution based design of proteins. *Methods in Enzymology* (523):213. <http://dx.doi.org/10.1016/B978-0-12-394292-0.00010-2>
17. **K.A. Reynolds**, R.N. McLaughlin, R. Ranganathan (2011). Hotspots for allosteric regulation on protein surfaces. *Cell* (147):1564. <http://dx.doi.org/10.1016/j.cell.2011.10.049>
18. M.S. Hanes, **K.A. Reynolds**, C. McNamara, P. Ghosh, R.A. Bonomo, J.F. Kirsch, T.M. Handel (2011). Specificity and cooperativity at β -lactamase position 104 in TEM-1/BLIP and SHV-1/BLIP interactions. *Proteins* (73):1267. <http://dx.doi.org/10.1002/prot.22961>
19. **K.A. Reynolds**, V. Katritch, R. Abagyan (2010). Structure and modeling of GPCRs: Implications for drug discovery. *Molecular Pharmacology and Drug Targeting: Shifting Paradigms and New Directions*, Ed. Annette Gilchrist, Chapter 15.
20. V. Katritch, **K.A. Reynolds**, V. Cherezov, M.A. Hanson, C.B. Roth, M. Yeager. R. Abagyan (2009). Analysis of full and partial agonists binding to β_2 -adrenergic receptor suggests a role of transmembrane helix V in agonist-specific conformational changes. *Journal of Molecular Recognition* (22):307. <http://onlinelibrary.wiley.com/doi/10.1002/jmr.949/abstract>
21. **K.A. Reynolds**, V. Katritch, R. Abagyan (2009). Identifying conformational changes of the β_2 adrenoceptor that enable accurate prediction of ligand/receptor interactions and screening for GPCR modulators. *Journal of Computer Aided Molecular Design* (23):273. <http://www.ncbi.nlm.nih.gov/pmc/articles/PMC2667566/?tool=pubmed>
22. **K.A. Reynolds**, M.S. Hanes, J.M. Thomson, A.J. Antczak, J.M. Berger, R.A. Bonomo, J.F. Kirsch and T.M. Handel (2008). Computational redesign of the SHV-1 β -lactamase/ β -lactamase Inhibitor Protein interface. *Journal of Molecular Biology* (382):1265. <http://dx.doi.org/10.1016/j.jmb.2008.05.051>
23. A.B. Chowdry, **K.A. Reynolds**, M.S. Hanes, M. Voorhies, N. Pokala, and T.M. Handel (2007). An object-oriented Library for Computational Protein Design. *Journal of Computational Chemistry* (28):2378. <http://onlinelibrary.wiley.com/doi/10.1002/jcc.20727/abstract>
24. **K.A. Reynolds**, J.M Thomson, K.D. Corbett, C.R. Bethel, J.M. Berger, J.F. Kirsch, R.A. Bonomo, and T.M. Handel (2006). Structural and Computational Characterization of the SHV-1 β -lactamase/ β -lactamase Inhibitor Protein (BLIP) interface. *Journal of Biological Chemistry* (281):26745. <http://www.jbc.org/content/281/36/26745.long>
25. M.A. Lovato, M.M. Meyer, **K.A. Foster**, W. K. Wilson, W. Gu, E. L. de Hostos, and S. P. T. Matsuda (2000). Cloning and characterization of the Dictyostelium discoideum cycloartenol synthase cDNA. *Lipids* (36):249. <http://dx.doi.org/10.1007/s11745-000-0520-3>

Funding

Current

NSF Modulus 8/2022-7/2025
Quantifying the prevalence and phenotypic consequences of transcriptional irreversibility in bacteria
\$1,093,791, Role: PI

NSF CAREER 6/2020 – 5/2025
CAREER: Defining structural principles for the engineering and evolution of allostery
\$1,099,999, Role: PI

NIH R01 4/2020 – 3/2024
Mapping genetic variation in enzyme velocity to growth rate phenotype
\$1,269,837, Role: PI

Completed

Gordon and Betty Moore Foundation, Data Driven Discovery Award Continuation 12/2019 – 11/2021
Decoding the genome using evolutionary statistics
\$350,000, Role: PI

Gordon and Betty Moore Foundation, Data Driven Discovery Award 12/2014 – 11/2019
Decoding the genome using evolutionary statistics
\$1.5M, Role: PI

Gordon and Betty Moore Foundation, Scialog Fellow Grant 7/2016 – 7/2017
Conditional Gene Essentiality as a Function of Cell Metabolic State
\$56,250, Role: PI

Teaching

Classroom Instruction

Thread head, Core Course thread in Computational and Systems Biology	2018-pres
Lecturer, Quantitative Biology, UTSW	2018-pres
Lecturer, Core course thread in Protein biophysics	2019-2021
Course director, Mathematical Foundations of Quantitative Biology, UTSW	2016-pres
Lecturer, Molecular Microbiology graduate course, UTSW	2014-2018
Lecturer, Core Course thread in Computational and Systems Biology	2013-2017
Lecturer, Mathematics in Medicine (a course for MD students), UTSW	2017
Discussion leader, Core Course - Proteins thread, UTSW	2015
Discussion leader, Molecular Microbiology journal club, UTSW	2015
Discussion leader, Core Course thread in Computational and Systems Biology	2014-2021
Bioinformatics outreach talk, UTSW STARS program	2014

Teaching related service

Member: *Molecular Biophysics graduate program,*
Biomedical Engineering graduate program, Computational Biology track.
Affiliated with Molecular Microbiology graduate program,, 2014-Fall 2018.

STARS Python workshop leader	2022-pres
Bioinformatics DEI Committee	2022-pres
DBS Graduate Student Admissions Committee	2020-pres

Chair, Computational Biology Curriculum Committee	2020-pres
Molecular Biophysics Steering Committee	2017-pres
Molecular Biophysics T32 Advisory Committee	2017-pres
SURF (summer undergraduate research fellowship) mentor, UTSW	2014-pres
Organizer, Comp/Sys Bio student WIPS series (w/ Jaqaman), UTSW	2015-2020
External reviewer, PhD thesis Matt Deyell, Paris Diderot, France	2018
Women in Science and Medicine (WISMAC) lunch panelist, UTSW	2017
Judge, Dallas Regional Science and Engineering Fair	2013-2017
Research mentor, Medical Student Summer Research Program	2015-2016
Green Center for Systems Biology Faculty Search Committee, UTSW	2014-2015
Research mentor, UT Dallas undergraduate senior thesis project	2011-2012
Women in Science and Engineering (WISE) mentor, SMU, Dallas TX	2008

Thesis committees: Zachary Markham, Ilona Gaszek (chair), Carla Madrid, Ashley Vu (chair), James Elder, Jesus Vega-Lugo (chair), Mike Trenfield (chair), Nick Lesner (chair), Leigh Manley, Paul Blazek (chair), Yusuf Tamer (chair)

Qualifying exam committees: Ashley Vu, Jesus Vega-Lugo, Mike Trenfield, Nick Lesner (chair), Michael Cotton, Paul Blazek (chair), Yusuf Tamer (chair), Bradley Quade

External Service

Ad hoc reviewer, NSF Chemistry of Life program, Molecular Biophysics program	2022
NIH ZRG1 GGG-P ML Member Conflict Genes, Genomes, and Genetics Study Section	2021
Organizer and publication committee chair for the Function Community of Special Interest, Intelligent Systems for Molecular Biology (ISMB) annual meeting.	2019-pres
Reviewer, Human Frontier Science Program (HFSP)	2019
Panelist, Board Meeting of the Research Corporation for Scientific Advancement	2018

Reviewer for: Science, eLife, Journal of Molecular Biology, Biophysical Journal, Nature Ecology and Evolution, Molecular Systems Biology, Nature Communications, Cell Systems, Nature Biotechnology, Structure, Molecular Biology and Evolution, PLOS Biology, Bioinformatics, Journal of Antimicrobial Chemotherapy, and Protein Science

Talks

2022

- 11/22 The genetic landscape of a metabolic interaction. Seminar, Department of Chemistry and School of Pharmacy, University of North Carolina. Chapel Hill, NC
- 09/22 A continuous epistasis model for predicting growth rate given combinatorial variation in gene expression and environment. Telluride Science Research Center Workshop on Emergent Simplicity in Biophysical Dynamics. Telluride, CO
- 09/22 The genetic landscape of a metabolic interaction. Seminar, Department of Biochemistry and Biophysics, Texas A&M University. College Station, TX
- 03/22 The genetic landscape of a metabolic interaction. Seminar, Department of Chemistry, University of Washington. Seattle, WA
- 02/22 Mapping the sequence determinants of protein regulation. Invited talk, Biopolymers *in vivo* subgroup, Biophysical Society. San Francisco, CA

2021

- 11/21 Mapping the sequence determinants of protein function and regulation. Harvard Systems Biology Theory Lunch (virtual)

- 11/21 Quantifying (and modeling) the relationship between gene expression and bacterial growth rate. Seminar, Department of Microbiology, UT Southwestern Medical Center
- 09/21 Challenges in synthesizing Deep Mutational Scanning data. Invited speaker and panelist, NSF workshop: Challenges and Opportunities in Synthesizing Massively Parallel Assays (virtual)
- 09/21 Understanding and using SCA. Invited workshop for the Herschlag and Fordyce labs, Stanford, CA (virtual)
- 07/21 Emergent simplicity in epistasis. Telluride Science Research Center workshop – Emergent simplicity in Biophysical Dynamics, Telluride, CO (virtual)
- 04/21 Mapping sequence constraints in an essential metabolic enzyme. Keynote speaker, Mutational Scanning Symposium, Center for the Multiplex Assessment of Phenotype, University of Washington (virtual)
- 03/21 Evolution inspired engineering of allostery. Seminar, Systems Biology, Universite Laval, Quebec CA (virtual)
- 2020**
- 10/20 Structurally distributed surface sites tune allosteric regulation. Seminar, Biological Physics, Arizona State University, Tempe AZ (virtual)
- 02/20 Mapping and modeling functional constraints on an essential metabolic enzyme. Invited speaker, Winter Q-Bio Annual Meeting, Waikoloa, HI
- 2019**
- 11/19 A two-enzyme adaptive unit within bacterial folate metabolism. Seminar, Center for Physics of Evolving Systems, University of Chicago, IL
- 07/19 Rewiring how cells respond to the environment, using protein sequence information. QP SURF lunch talk, UTSW, Dallas, TX
- 06/19 Hotspots for the evolution and engineering of allosteric regulation. Invited speaker, Molecular mechanisms in evolution Gordon Research Conference, MA
- 05/19 A two-enzyme adaptive unit within bacterial folate metabolism. UC Irvine, CA
- 04/19 Comprehensively mapping the mutations influencing allostery in a model enzyme. Stanford University, CA
- 04/19 Rewiring how cells respond to the environment, using protein sequence information. Gordon and Betty Moore Investigator Symposium, San Francisco, CA
- 03/19 Hotspots for the evolution and engineering of allosteric regulation. Invited speaker, Biophysical Society, Baltimore, MD
- 2018**
- 12/18 Hotspots for the evolution and engineering of allosteric regulation. Invited speaker, ASCB annual meeting, San Diego, CA
- 10/18 Hotspots for the evolution and engineering of allosteric regulation. Invited speaker, Northeastern Structure Symposium, Farmington, CT
- 07/18 Using evolutionary information to understand cellular systems. Keynote speaker, Function COSI – ISMB annual meeting, Chicago, IL
- 06/18 Evolution and engineering of allosteric regulation in protein kinases. Invited speaker, Protein Engineering Canada, Vancouver, CA
- 03/18 Using genomic data to identify modularity in cell systems. Invited speaker, Biology seminar series, Texas A&M University, College Station, TX
- 01/18 Genotype, phenotype. Gordon and Betty Moore Investigator Symposium, Monterey, CA

2017

- 10/17 Decoding the genome with evolutionary statistics. Keynote speaker, Australasian Genomic Technologies Association (AGTA) Conference, Hobart, Tasmania.
- 10/17 Using evolutionary information to decode the genome. Invited speaker, BioResearch Conference, UT Dallas, Dallas, TX
- 09/17 Hotspots for the evolution and engineering of new allostery. MSTP works in progress talk, UTSW, Dallas, TX
- 07/17 Hotspots for the evolution and engineering of allosteric regulation. Invited speaker, Workshop on designing biomolecular switches, Telluride Science Research Center, Telluride, CO
- 06/17 Using genomic data to identify modularity in cell systems. QP SURF lunch talk, UTSW, Dallas, TX
- 04/17 Conditional gene essentiality as a function of cell metabolic state. Funding awardee, Scialog Molecules-Come to-Life meeting, Tuscon, AZ
- 03/17 Evolutionary modularity. Invited speaker, Quantitative Biosciences Institute Spring Mutations meeting, UCSF, San Francisco, CA
- 03/17 An evolutionary module in central metabolism. Invited speaker, qBio seminar series, UCSD, San Diego, CA
- 02/17 Evolution of regulatory diversity in the kinase superfamily. Platform Talk, Biophysical Society Annual Meeting, New Orleans.
- 01/17 An evolutionary module in central metabolism. Student-invited speaker, Bioinformatics Biophysics and Chemistry (BBC) seminar. University of California, San Francisco.

2016

- 10/16 Statistical Genomics. Gordon and Betty Moore Investigator Symposium, New York, NY.
- 04/16 A conserved evolutionary module in central metabolism. Invited speaker, Biophysics seminar, ESPCI Paris Tech, Paris, France.
- 03/16 An evolutionary module in central metabolism. Invited speaker, Biophysics seminar, University of Illinois, Urbana-Champaign
- 03/16 An evolutionary module in central metabolism. Invited speaker, Biochemistry and molecular biology graduate student hosted seminar, University of British Columbia, Vancouver, Canada.

2015

- 11/15 A statistical genomics approach to understanding cellular systems. Mathematics and biology seminar series, Southern Methodist University, (Dallas, TX)
- 10/15 Decoding the genome: Relating sequence variation to function and phenotype. Gordon and Betty Moore Investigator Symposium, (Seattle, WA)
- 08/15 An evolutionary module in central metabolism. Endowed scholars WIPS, UTSW (Dallas, TX)
- 08/15 Hotspots for allosteric regulation on a protein surface. Evolutionary Cell Biology Program, Kavli Institute for Theoretical Physics, UCSB (Santa Barbara, CA)
- 08/15 Decomposing complex systems. Evolutionary Cell Biology Program, Kavli Institute for Theoretical Physics, UCSB (Santa Barbara, CA)
- 05/15 Decomposing complex systems. Guest lecturer, Howard Berg lab, Harvard (Boston, MA)

2014

- 12/14 Using evolutionary statistics to find functional modules. Invited talk, MIT (Boston, MA)
- 12/14 Finding evolutionary “design principles” for cellular systems. Special biophysics seminar, Boston University (Boston, MA)
- 11/14 Using evolutionary statistics to find functional modules. Microbiology seminar, UTSW (Dallas, TX)

- 09/14 Using evolutionary statistics to find functional modules. Molecular Biophysics discussion group, UTSW (Dallas, TX)
- 09/14 Understanding Cellular Systems Using Genome Data. UTSW STARS program – public science talks for educators (Dallas, TX)
- 09/14 Decoding the genome. New Faculty Research Forum, UTSW (Dallas, TX)
- 07/14 Decoding the genome. Invited talk, Gordon and Betty Moore Foundation data driven discovery finalist symposium (San Jose, California)
- 06/14 Principles of function in cellular protein networks. Invited talk, Protein Engineering Canada Conference (Ottawa, Ontario)

2013

- 12/13 Principles of function in cellular protein networks. Graduate student invited seminar, UTHSC (Houston, TX)
- 09/13 Evolution, engineering and epistasis: mapping functional coupling between proteins. Seminar, MRC Laboratory of Molecular Biology (Cambridge, England).
- 02/13 Principles of function in cellular protein networks. Special seminar, Dept. of Bioengineering, California Institute of Technology (Pasadena, CA).
- 02/13 Principles of function in cellular protein networks. Special seminar, Dept. of Biochemistry, Molecular Biology and Biophysics, University of Minnesota (St. Paul, MN).
- 02/13 Principles of function in cellular protein networks. Special seminar, FAS Center for Systems Biology, Harvard University (Cambridge, MA).
- 02/13 Principles of function in cellular protein networks. Special seminar, Dept. of Systems Biology, Harvard Medical School (Boston, MA).
- 01/13 Principles of function in cellular protein networks. Special seminar, Green Center for Systems Biology, UTSW Medical Center (Dallas, TX)

2012

- 12/12 Principles of function in cellular protein networks. Earl Stadtman Symposium on genetics, genomics and systems biology, NIH (Bethesda, MD)
- 11/12 Principles of function in cellular protein networks. Special seminar, Dept. of Biology, Amherst College (Amherst, MA).
- 07/12 A structural model for the emergence of allosteric control in proteins. Gordon Research Conference, Intrinsically Disordered Proteins (Mount Snow, VT)
- 02/12 Hotspots for allosteric regulation on a protein surface. Finalist interview talk, UTSW award for excellence in postdoctoral research (Dallas, TX).
- 01/12 Hotspots for allosteric regulation on a protein surface. Seminar, Dept of Systems Biology, Harvard Medical School (Boston, MA).

2009-2011

- 07/11 Hotspots for allosteric regulation on a protein surface. Gordon Research Conference, Mechanisms of Cell Signaling (Bates College, ME).
- 03/11 A structural model for the emergence of allosteric control in proteins. Annual Meeting of the American Physical Society. (Dallas, TX)
- 02/11 A mechanism for the evolution of regulation in proteins. Invited talk, Biophysics group, CNRS (Grenoble, France)
- 10/10 A mechanism for the evolution of allosteric control in proteins. Dutch meeting on Molecular and Cellular Biophysics (Veldhoven, Netherlands).
- 03/10 Evolution of Allosteric Regulation in Proteins. Protein allostery meeting, UCSD. (San Diego, CA)
- 10/09 Evolution-based engineering of allosteric regulation in proteins. Society for Neuroscience (Chicago, IL).