DEEPTI KARANDUR

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Education

2008-2015 – Ph.D. SCBMB, Baylor College of Medicine. Advisor: B. Montgomery Pettitt

2004-2006 – M.Sc. in Bioinformatics, Madras University (Graduated with Distinction)

2001-2004 – B.Sc. in Chemistry, Botany and Microbiology, Bangalore University

Research/Work Experience

October, 2025 – present – Angreal Research

- Adapting newly-developed machine learning methods such as DeepMindMD to accelerate the sampling of conformational space accessible to proteins during simulations.

- Co-PI (with Neel Shah) on a supercomputing allocation at the San Diego Supercomputing Center.

October, 2022 – present – Independent Research

- Collaboration with the Neel Shah Lab at Columbia University to understand how mutations in the tyrosine phosphatase SHP2 affect its activity.
  These studies have resulted in multiple publications including in PNAS and Nature Communications

July, 2023 – June,2024 – Research Instructor, John Kuriyan Group, Vanderbilt University School of Medicine

- Adapting newly-developed protein design methods such as ProteinMPNN to design variants of cell signaling proteins in order to understand their structure-function relationships.

March, 2015 – June, 2022 – Post-doctoral Research Associate, John Kuriyan Group, Howard Hughes Medical Institute at University of California, Berkeley

- Used molecular dynamics simulations and enhanced sampling methods to understand the mechanism of transmission of signal in EGFR from the extracellular receptor module to the intracellular catalytic domain, across the membrane.
  This work led to a publication in eLife

- Used long timescale all-atom molecular dynamics simulations, run on the special-purpose supercomputer Anton2, to elucidate the role of the regulatory segment in activation-dependent hub disassembly of CaMKII
  This work led to a publication in eLife

- Used coarse-grained molecular dynamics simulations to determine the mechanism of activation kinetics of the Arf/GEF complex on the membrane
  This work led to a publication in PNAS that was highlighted by a Commentary written at the invitation of the Editorial Board of PNAS

2008 - 2015 – Ph.D. SCBMB, Baylor College of Medicine. Advisor B. Montgomery Pettitt

- Used all-atom molecular dynamics simulations and thermodynamic integration free energy calculations to study the solubility and aggregation of oligoglycines in water

Publications

1. A. E. van Vlimmeren, Z. Jiang, **D. Karandur**, A.T. Applebaum Licht, N. H. Shah, "The pathogenic E139D mutation stabilizes a non-canonical active state of the multi-domain phosphatase SHP2"; Protein Sci; 2025; 34(12); e70373

2. Z. Jiang, A. E. van Vlimmeren, **D. Karandur**, A. Semmelman, N. H. Shah, "Deep mutational scanning of a multi-domain signaling protein reveals mechanisms of regulation and pathogenicity"; Nature Communications; 2025; 16(1), 5464

3. A. E. van Vlimmeren, R. Voleti, C. A. Chartier, Z. Jiang, **D. Karandur**, N. H. Shah, "The pathogenic T42A mutation in SHP2 rewires interaction specificity and enhances signaling"; Proc. Natl. Acad. Sci. USA; 2024; 121 (30); e2407159121

4. F. Hidalgo, L. M. Nocka, N. H. Shah, K. Gorday, N. R. Latorraca, P. Bandaru, S. Templeton, D. Lee, **D. Karandur**, J. G. Pelton, S. Marqusee, D. Wemmer, J. Kuriyan, "A saturation-mutagenesis analysis of the interplay between stability and activation in Ras"; eLife; 2022; 11; e76595

5. Y. Huang, J. Ognjenovic, **D. Karandur**, K. Miller, A. Merk, S. Subramaniam, J. Kuriyan, "A molecular mechanism for the generation of ligand-dependent differential outputs by the epidermal growth factor receptor"; eLife; 2021; 10: e73218

6. **D. Karandur***, M. Bhattacharyya*, Z. Xia*, Y. K. Lee, S. Muratcioglu, E. McSpadden, B. Qiu, J. Groves, E. Williams, J. Kuriyan, "Breakage of the Oligomeric CaMKII Hub by the Regulatory Segment of the Kinase"; eLife; 2020; 9: e57784

7. J. C. Cofsky, **D. Karandur**, C. J. Huang, I. P. Witte, J. Kuriyan, J. A. Doudna, "CRISPR-Cas12a exploits R-loop asymmetry to form double-strand breaks"; eLife, 2020; 9: e55143

8. M. Bhattacharyya, **D. Karandur**, and J. Kuriyan, "Structural Insights into the Regulation of Ca2+/Calmodulin-Dependent Protein Kinase II (CaMKII)"; Cold Spring Harb. Perspect. Biol.; 2020; 2 (6), a035147

9. Y. Kondo*, J. Ognjenović, S*. Banerjee, **D. Karandur**, A. Merk, K. Kulhanek, K. Wong, J. P. Roose, S. Subramaniam, J. Kuriyan, "Cryo-EM structure of a dimeric B-Raf: 14-3-3 complex reveals asymmetry in the active sites of B-Raf kinases"; Science; 2019; 366 (6461), 109

10. **D. Karandur***, A. Nawrotek*, J. Kuriyan, J. Cherfils, "Multiple Interactions Between an Arf/GEF Complex and Charged Lipids Determine Activation Kinetics on the Membrane."; Proc. Natl. Acad. Sci. USA; 2017; 114(43); 11416. (This paper was highlighted by a Commentary written at the invitation of the Editorial Board of PNAS.)

11. D. Asthagiri, **D. Karandur**, D. S. Tomar, B. M. Pettitt, "Intramolecular Interactions Overcome Hydration to Drive the Collapse Transition of Gly15."; J. Phys. Chem. B., 2017; 121(34); 8078

12. N. H. Shah, Q. Wang, Q. Yan, **D. Karandur**, T. Kadlecek, I. R. Fallahee, W. P. Russ, R. Ranganathan, A. Weiss, J. Kuriyan; "An Electrostatic Selection Mechanism Controls Sequential Kinase Signaling Downstream of the T Cell Receptor"; eLife, 2016; 5: e20105

13. Y. Huang*, S. Bharill*, **D. Karandur**, S. M. Peterson, M. Maritia, X. Shi, M. J. Kaliszewski, A. W. Smith, E. Isacoff, J. Kuriyan; "Molecular Basis for Multimerization in the Activation of the Epidermal Growth Factor Receptor"; eLife, 2016; 5: e14107

14. **D. Karandur**, B. M. Pettitt, "The Contribution of Electrostatic Interactions to the Collapse of Oligoglycine in Water"; Condens. Matter. Phys., 2016; 19(2); 23802

15. **D. Karandur**, R. Harris, B. M. Pettitt, "Protein Collapse Driven Against Solvation Free Energy, Without H-bonds"; Protein Sci., 2016; 25(1); 103

16. **D. Karandur**, K-Y. Wong, B. M. Pettitt, "Solubility and Aggregation of Gly_5 in Water"; J. Phys. Chem. B., 2014; 118(32); 9565

17. A. Marathe, **D. Karandur**, M Bansal; "Small local variations in B-form DNA lead to a large variety of global geometries which can accommodate most DNA-binding protein motifs", BMC Structural Biology; 2009; 9(1); 24

*contributed equally to this work

Mentoring & Teaching Experience

Co-ordinator – Undergraduate Research at the Kuryian Lab 2017-2021

- Responsible for recruiting students to the undergraduate research program in the lab (usually between 9-12 undergraduate student researchers at any point).
- Mentoring students through undergraduate research projects, providing guidance with issues with their projects, etc.
- Ensuring students are aware of opportunities for internships, fellowships, awards, etc. and helping them put together applications for them

Mentoring

Thu Nguyen, undergraduate student in Chemistry, Vanderbilt University	2023-2024
Kate Miller, undergraduate student in Molecular and Cell Biology, UC Berkeley Currently a graduate student at Stanford University	2020-2021
Chaz Sykes, undergraduate student in Mathematics and Physics, UC Berkeley	2018-2020
Chris Chi, undergraduate student in Chemical Biology, UC Berkeley Currently a graduate student at University of Chicago (Aaron Dinner group)	2018-2019
Peter Ren, undergraduate student in Chemical Biology, UC Berkeley Currently a graduate student at Harvard University	summer, 2018
Adam Stein, undergraduate student in Physics, UC Los Angeles	summer, 2018
Sarah Mulchand, undergraduate student in Molecular and Cell Biology, UC Berkeley Currently at Dragoneer Investment Group, San Francisco	2017-2018
Andrew Low, undergraduate student in Computer Science, UC Berkeley Currently a Research Associate at UC Berkeley	2016-2017
Tomer Rotstein, undergraduate student in Bioengineering UC Berkeley Currently a graduate student at Duke University (Xiling Shen group)	2015-2016

Teaching

Guest Lecturer, Biophysical Chemistry: Physical Principles and the Molecules of Life at UC Berkeley
Upper division undergraduate course covering thermodynamic and kinetic concepts applied to understanding the chemistry and structure of biomolecules

Presentations

Talks

"Activation-Triggered Hub Disassembly in CaMKII", Division of Biochemistry, Biophysics & Structural Biology Retreat, Asilomar, January 2019

"Understanding Allostery in Ras Through Computational and Structural Methods" UC Berkeley Structure Supergroup Seminar, Berkeley, November 2018

"Membrane-Dependent Activation of Arf/GEF Complexes" Berkeley Graduate Group Retreat, Berkeley, October 2017

"Protein Folding and Collapse: Aggregation of Oligoglycine" Structural and Computational Biology and Molecular Biophysics Annual Research Conference and Retreat, Houston, January 2013, Houston

Posters

"Mechanism of CaMKII Disassembly", Gordon Research Conference on Proteins, June 2019

"Protein Folding and Collapse: Thermodynamics of Aggregation of Gly_5 vs Concentration in Solution", 9th Annual Structural Biology Symposium, Sealy Center for Structural Biology and Molecular Biophysics, May 2014, Galveston (won award for best poster)

"Protein Folding and Collapse: Thermodynamics of Aggregation of Gly_5 vs Concentration in Solution", 58th Annual Meeting, Biophysical Society, February 2014, San Francisco

"Aggregation of Oligoglycine in Water", 21st Texas Protein Folders Meeting, March 2013, Camp Allen, Texas

Other Service and Outreach Activities

Panelist & Speaker, Undergraduate Research Q&A, Undergraduate Research Resilience Program, University of California, Berkeley

Early-career reviewer, *eLife*

Early-career reviewer, *Protein Science*

Early user/tester (by invitation) of several high-performance supercomputers including at Oakridge National Labs (Keeneland, Titan), Texas Advanced Supercomputing Center (Frontera) and Pittsburg Supercomputing Center (Bridges2)

Podcast on using high-performance computers to study the structure-function relationships of B-Raf, a protein implicated in 80% of melanomas

Talk at the Berkeley Cloud Computing Meetup on using high performance computers to study the structure-function relationships in cancer proteins