Paul Robustelli, Ph.D. **Assistant Professor of Chemistry**
Paul.J.Robustelli@Dartmouth.edu **Dartmouth College**

Education

- **University of Cambridge** - Ph.D. in Chemistry (2010)
  - Dissertation Title: Protein Structure Determination from NMR Chemical Shifts
  - Supervisor: Prof. Michele Vendruscolo
- **Pomona College** - B.A. in Chemistry with Minor in Mathematics (2006)

Professional Experience

- **Dartmouth College (Jan 2020–Present)**
  Assistant Professor of Chemistry
  - Member, Neukom Faculty Cluster of Computational Science
  - Member, Department of Biochemistry and Cell Biology
  - Member, Dartmouth Cancer Center
- **D.E. Shaw Research (2013-2019)**
  Scientist
  - Developing Improved Physical Models for the Accurate Simulation of both Folded and Disordered Protein States
  - Elucidating Dynamic Binding Modes of Small Molecules with Intrinsically Disordered Proteins and Rationally Designing Tighter Binders
- **Columbia University Medical Center (2010-2013)**
  NSF Postdoctoral Research Fellow
  - Mentor: Prof. Arthur G. Palmer III
  - Studying the Role of Conformational Dynamics in Protein Function with NMR Spectroscopy and Molecular Simulations
- **University of Cambridge, Department of Chemistry (2006-2010)**
  Graduate Research Assistant
  - Mentor: Prof. Michele Vendruscolo
  - Development and Application of Novel Computational Methods for Protein Structure Determination from NMR Chemical Shifts
- **Pomona College, Department of Chemistry (2004-2006)**
  Undergraduate Research Assistant
  - Mentor: Prof. Wayne E. Steinmetz
  - Determination of the Structure and Conformational Dynamics of Tricothecene Mycotoxins with NMR Spectroscopy and Molecular Modeling

Manuscript Preprints Under Review:

1. Structure-Based Experimental Datasets for Benchmarking of Protein Simulation Force Fields. CE Cavender, DA Case , JC Chen, LT Chong, DA Keedy, K Lindorff-Larsen , DL Mobley , OH Ollila, C Oostenbrink, P Robustelli, VA Voelz, ME Wall, DC Wych, MK Gilson. *arXiv* (2023) doi: https://doi.org/10.48550/arXiv.2303.11056

Peer Reviewed Publications (Total: 25, Total Citations: 3292, h-index: 18, i-10 index: 21, i-100 index: 8)
Google Scholar Page: https://scholar.google.com/citations?user=2Fr4owoAAAAJ&hl=en

1. Folding-upon-binding Pathways of an Intrinsically Disordered Protein from a Deep Markov State Model. T Sisk, P Robustelli, *Proceedings of the National Academy of Sciences*, *121*(6), p.e231336012 (2024)

2. PED in 2024: improving the community deposition of structural ensembles for intrinsically disordered proteins. Ghafouri, H., Lazar, T., Del Conte, A., Ku, PED Consorium, P. Robustelli, L.G.T., Aspromonte, M., Bernadó, P., Chaves-Arquero, B., Chemes, L.B., Clementel, D., Cordeiro, T. and Elena-Real, C., *Nucleic acids research*, *52*(D1), pp.D536-D544. (2024)

3. Rational optimization of a transcription factor activation domain inhibitor. S. Basu, P. Martinez-Cristoabl, M. Pesarrodona, M. Frigole-Viva, E. Szulc, M. Lewis, A. Banuelos, C. Sanchexz-Zarzalego, S. Bielskute, J. Zhu, C. Garcia-Cabau, C. Batlee, B. Mateos, M. Biesaga, A. Escobedo, L. Bardia, X. Verdaguer, A. Ruffoni, N.R. Mawji, J. Wang, T. Tam, I. Brun-Heath, S. Ventura, D. Meierhofer, J. Garcia, P. Robustelli, T.H. Stracker, M.D. Sadar, A. Riera, D. Hnisz, X. Salvatella, *Nature Structural and Molecular Biology 30*(12), pp.1958-1969. (2023)

4. Clustering conformational ensembles of intrinsically disordered proteins with t-distributed stochastic neighbor embedding. R Appadurai, JK Koneru, M Bonomi, P Robustelli*, A Srivastava* (*=co-corresponding authors). *Journal of Chemical Theory and Computation,* 19, 14, 4711–4727 (2023)

5. Dissecting the biophysics and biology of intrinsically disordered proteins. PR Banerjee, R Priya , AS Holehouse, R Kriwacki, P Robustelli, H Jiang, AI Sobolevsky, JM Hurley, and JT Mendell. *Trends in Biochemical Sciences* (2023)

6. Small Molecules Targeting the Disordered Transactivation Domain of the Androgen Receptor Induce the Formation of Collapsed Helical States, J. Zhu, X. Salvatella, P. Robustelli, *Nature Communications,* 13 (1), 1-15 (2022)

7. Molecular basis of small-molecule binding to a-synuclein, P Robustelli, Ibanez-de-Opakua A, Campbell-Bezat C, Giordanetto F, Becker S, Zweckstette Mr, Pan AC, Shaw DE, *Journal of the American Chemical Society*, 144, 6, 2501-2519 (2022)

8. Quantifying the Relationship between Conformational Dynamics and Enzymatic Activity in Ribonuclease HI Homologues, J Martin, P Robustelli, AG Palmer III, *Biochemistry*, 59 (35), 3201-3205 (2020)

9. The Mechanism of Coupled Folding-Upon-Binding of An Intrinsically Disordered Protein, P Robustelli, S Piana, DE Shaw, *Journal of the American Chemical Society,* 142 (25), 11092-11101 (2020)

10. Development of a Force Field for the Simulation of Single-Chain Proteins and Protein-Protein Complexes. S Piana*, P Robustelli*, D Tan, S Chen, DE Shaw (*=equal contributions), *Journal of Chemical Theory and Computation*, 16, 4, 2494-2507 (2020)

11. Developing a Molecular Dynamics Force Field for Both Folded and Disordered Protein States, P Robustelli, S Piana, DE Shaw, *Proceedings of the National Academy of Sciences*, p.201800690 (2018)

12. Water Dispersion Interactions Strongly Influence Simulated Structural Properties of Disordered Protein States, S Piana, A Donchev, P Robustelli, DE Shaw, *Journal of Physical Chemistry B,* 119 (16), 5113-5123 (2015)

13. Functional implications of large backbone amplitude motions of the glycoprotein 130-binding epitope of interleukin-6, R Bobby, P Robustelli, AV Kralicek, M Mobli, GF King, J Grötzinger, AJ Dingley, *FEBS Journal,* 281(10), 2471-83 (2014

14. Conformational Dynamics of the Partially Disordered Yeast Transcription Factor GCN4, P Robustelli, N Trbovic, RA Friesner, AG Palmer III, *Journal of Chemical Theory and Computation*, 9(11), 5190–5200 (2013)

15. Thermal Adaption of Conformational Dynamics in Ribonuclease H, KA Stafford, P Robustelli, AG Palmer III, *PLoS Computational Biology*, 9(10), e1003218 (2013)

16. Structure of an Intermediate State in Protein Folding and Aggregation, P Neudecker, P Robustelli, A Cavalli, P Walsh, P Lundstrom, A Zarrine-Afsar, S Sharpe, M Vendruscolo, LE Kay, *Science*, 336, 362-366 (2012)

17. Interpreting Protein Structural Dynamics from NMR Chemical Shifts, P Robustelli, KA Stafford, AG Palmer III, *Journal of the American Chemical Society*, 134, 6365-6374 (2012)

18. Characterization of the Conformational Equilibrium Between the Two Major Substates of RNase A using NMR chemical shifts, C Camilloni, P Robustelli, A De Simone, A Cavalli, M Vendruscolo, *Journal of the American Chemical Society*, 134, 3968-3971 (2012)

19. Effects of the Known Pathogenic Mutations on the Aggregation Pathway of the Amyloidogenic Peptide of Apolipoprotein A-I, S Raimondi, F Guglielmi, S Giorgetti, S Di Gaetano, A Arciello, DM Monti, A Relini, D Nichino, SM Doglia, A Natalello, P Pucci, P Mangione, L Obici, G Merlini, M Stoppini, P Robustelli, GG Tartaglia, M Vendruscolo, CM Dobson, R Piccoli, V Bellotti, *Journal of Molecular Biology*, 407(3), 465-76 (2011)

20. Using NMR Chemical Shifts as Structural Restraints in Molecular Dynamics Simulations of Proteins, P Robustelli, KJ Kohlhoff, A Cavalli, M Vendrusculo, *Structure*, 18, 1-11 (2010)

21. Fast and Accurate Predictions of Protein NMR Chemical Shifts from Interatomic Distance, KJ Kohlhoff, P Robustelli, A Cavalli, X Salvatella, M Vendruscolo, *Journal of the American Chemical Society,* 131 (39), 13894-13895 (2009)

22. Folding of Small Proteins with Chemical Shift Restrained Monte Carlo Simulations without the use of Molecular Fragment Replacement or Structural Homology, P Robustelli, A Cavalli, CM Dobson, M Vendruscolo, X Salvatella, *Journal of Physical Chemistry B,* 113 (22), 7890-7896 (2009)

23. Determination of Protein Structures in the Solid State from NMR Chemical Shifts, P Robustelli, A Cavalli, M Vendruscolo, *Structure*, 16, 1764-1769 (2008)

24. Structure and Conformational Dynamics of Tricothecene Mycotoxins, WE Steinmetz, P Robustelli, E Edens, D Heineman, *Journal of Natural Products*, 71 (4), 589-594 (2008)

25. A Molecular switch based on a biologically important redox reaction, P Yan, MW Holman, P Robustelli, A Chowdhury, FI Ishak, DM Adams, *Journal of Physical Chemistry B*, 109, 130-137 (2005)

Funding Awarded

- Cottrell Scholar Award Scholar Award (2024) – PI
    - "Characterizing and modulating interactions of disordered proteins that drive biomolecular condensate formation and cytotoxic aggregation"
    - Total Award: $120,000 (Direct Costs)

- Nuage Therapeutics Sponsored Research Agreement (2023) - PI
    - "Characterizing the binding modes of small molecules that modulate biomolecular condensate formation to inform the design of cancer therapeutics"
    - Total Award: $250,000 (Direct Costs) / $260,000 (Total Costs)
- Dartmouth Innovations Accelerator for Cancer (DIAC) Development Award (2022) - PI
    - "A Drug Design Platform for Disordered Proteins"
    - Total Award: $150,000 (Total Costs)
- Dartmouth Innovations Accelerator for Cancer (DIAC) Stu Trembly Award (2021) - PI
    - Total Award: $25,000 (Total Costs)
- NIH Maximizing Investigators Research Award (MIRA) – NIH#R35GM142750 (2021-2026) - PI
    - "Characterizing the binding mechanisms of castration-resistant prostate cancer therapeutics to the intrinsically disordered N-terminal domain of the Androgen Receptor"
    - Total Award: $1,250,000 (Direct Costs) / $1,979,921 (Total Costs)
- National Research Council/Pittsburgh Supercomputing Center Anton2 Supercomputing Grant - MCB200087P (2023) – PI
    - "Understanding the effects of 1,6-hexanediol on the properties of biomolecular condensates"
    - Total Award: 460,000 MD Simulation Unit
- National Research Council/Pittsburgh Supercomputing Center Anton2 Supercomputing Grant - MCB230012P (2023) – co-PI (PI: Prof. Brittany Morgan – Notre Dame University)
    - "Rationalizing Differences in the Reactivity and Site Selectivity of Covalent Ligands that Bind the Flexible, Multi-Domain heterogenous nuclear RiboNucleoProteins (hnRNPs) H and F"
    - Total Award: 460,000 MD Simulation Unit
- National Research Council/Pittsburgh Supercomputing Center Anton2 Supercomputing Grant -
- MCB200087P (2021) - PI
    - "Characterizing the binding mechanisms of castration-resistant prostate cancer therapeutics to the intrinsically disordered N-terminal domain of the Androgen Receptor"
    - Total Award: 460,000 MD Simulation Unit
- National Research Council/Pittsburgh Supercomputing Center Anton2 Supercomputing Grant - MCB200087P (2020) - PI
    - "Characterizing the binding mechanisms of castration-resistant prostate cancer therapeutics to the intrinsically disordered N-terminal domain of the Androgen Receptor"
    - Total Award: 460,000 MD Simulation Units
- Burke Research Initiation Award, Dartmouth College (2020-2022) – PI
    - Total Award: $35,000
- National Science Foundation Postdoctoral Research Fellowship - NSF#1002684 (2010-2012) – PI
    - Total Award: $123,000
- National Science Foundation Graduate Research Fellowship - NSF#0938784 (2006-2010)
    - Total Award: $124,500 ($41,500 accepted)
- Gates Cambridge Scholarship (2006-2009)
    - Total Award: $250,000

Oral Conference Presentations

1. "Targeting Intrinsically Disordered Proteins and Biomolecular Condensates with Small Molecule Drugs" Molecular Biophysics in the Northeast, Amherst, MA (2024)
2. "Molecular Recognition Mechanisms of Intrinsically Disordered Proteins" Protein Folding & Dynamics Gordon Research Conference, Galveston, TX (2024)
3. "Conformational Ensembles and Molecular Recognition Mechanisms of Intrinsically Disordered Proteins" American Chemical Society Fall Meeting, San Francisco, CA (2023)

4. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” Aqueous Supramolecular Chemistry Workshop, Bozeman, MT (2023)
5. “Conformational Ensembles and Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” Computational Aspects of Biomolecular NMR Gordon Research Conference, West Dover, VT (2023)
6. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” Prague Protein Spring Meeting, Prague, Czech Republic, (2023)
7. “Targeting Intrinsically Disordered Proteins and Biomolecular Condensates with Small Molecule Drugs” Understanding the Role of Intrinsically Disordered Proteins in Cancer Biology, National Cancer Institute Workshop, Rockville, MD, USA, Rockland, MD, USA (2022)
8. “How Do Small Molecule Drugs Bind Intrinsically Disordered Proteins?” 29th International Conference On Magnetic Resonance In Biological Systems, Boston, MA, USA (2022)
9. “How Do Small Molecule Drugs Bind Intrinsically Disordered Proteins?” Computational Chemistry Gordon Research Conference, Castelldefels, Spain (2022)
10. “How Do Small Molecule Drugs Bind Intrinsically Disordered Proteins?” Intrinsically Disordered Proteins Telluride Science Research Center Workshop, CO, USA (2021)
11. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” Open Source Software for Enhanced-Sampling Simulations, Lugano, Switzerland, (2019)
12. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” Biomolecules and Nanostructures, Pomlewo, Poland (2019)
13. “Improved Physical Models Enable the Investigation of Molecular Recognition in Intrinsically Disordered Proteins at Atomistic Resolution” - Biophysical Society Meeting, Baltimore, MD, USA (2019) Biophysical Society Meeting, Baltimore, MD, USA (2019)
14. “Improved Physical Models Enable the Investigation of Molecular Recognition in Intrinsically Disordered Proteins at Atomistic Resolution” Computational Biophysics at the Molecular and Mesoscales, Quy Nhon, Vietnam (2018)
15. “Improved Physical Models Enable the Investigation of Molecular Recognition in Intrinsically Disordered Proteins at Atomistic Resolution” Protein Society Meeting, Boston, MA, USA (2018)
16. “An Improved Force Field Enables the Elucidation of the Fundamental Biophysical Interactions of Intrinsically Disordered Proteins” CECAM Workshop: Disordered Protein Segments, Paris, France (2017)
17. “Developing Force Fields for the Accurate Simulation of Both Ordered and Disordered Protein States” Conformational Ensembles from Experimental Data and Computer Simulations, Berlin, Germany (2017)
18. “Developing Force Fields for the Accurate Simulation of Both Ordered and Disordered Protein States” Biophysical Society Meeting, New Orleans, LA, USA (2017)
19. “Developing Force Fields that More Accurately Describe the Structural Properties of Ordered and Disordered Protein States” Experimental Nuclear Magnetic Resonance Conference, Asilomar, CA, USA (2015)
20. “Tuning the Conformational Dynamics and Enzymatic Activity of Ribonuclease H” Frontiers of Structural Biology Keystone Symposia, Snowbird, UT, USA (2014)
21. “Atomistic Descriptions of Protein Dynamics on Multiple Timescales from NMR Chemical Shifts” Computational Aspects - Biomolecular NMR Gordon Research Conference, West Dover, VT, USA (2013)
22. “Atomistic Descriptions of Protein Dynamics on Multiple Timescales from NMR Chemical Shifts” ISMAR Meeting, Rio De Janiero, Brazil (2013)

23. “Dynamically Averaged NMR Chemical Shifts Provide Atomistic Descriptions of Protein Motions” Protein Society Meeting, Boston, MA, USA (2011)
24. “Direct Utilization of Chemical Shift Restraints in Protein Structure Calculations” Protein Society Meeting, Boston, MA, USA (2009)

Selected Invited Seminars

1. “Targeting Intrinsically Disordered Proteins and Biomolecular Condensates with Small Molecule Drugs”, Yale University, New Haven, CT (2024)
2. “Targeting Intrinsically Disordered Proteins and Biomolecular Condensates with Small Molecule Drugs”, Iowa State University, Ames, IA (2024)
3. “Targeting Intrinsically Disordered Proteins and Biomolecular Condensates with Small Molecule Drugs”, Notre Dame University, South Bend, IN (2023)
4. “Targeting Intrinsically Disordered Proteins and Biomolecular Condensates with Small Molecule Drugs”, Wesleyen University, Middlletown, CT (2023)
5. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”, Albert Einstein Medical College, New York, NY (2023)
6. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”, University of Virginia, Charlottesville, VA (2023)
7. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”, Tulane University, New Orleans, LA (2023)
8. “Targeting Intrinsically Disordered Proteins and Biomolecular Condensates with Small Molecule Drugs” Roivant Discovery, New York, NY, USA (2022)
9. “Maximum-Entropy Methods for Integrative Modeling of Disordered Proteins”, Indian Institute of Science Bangalore, Molecular Biophysics Unit, Integrative Modelling In Biophysics Seminar Series, Bangalore, India, (2022)
10. “How Do Small Molecule Drugs Bind Intrinsically Disordered Proteins?”, New Equilibrium Biosciences, IDP Conversations Seminar Series, Boston, MA, (2022)
11. “How Do Small Molecule Drugs Bind Intrinsically Disordered Proteins?”, Skidmore College, Saratoga Springs, NY (2022)
12. “How Do Small Molecule Drugs Bind Intrinsically Disordered Proteins?”, Spelmen College, Atlanta, GA, (2022)
13. “How Do Small Molecule Drugs Bind Intrinsically Disordered Proteins?”, Colby College, Watertownn, ME (2022)
14. “Characterizing dynamic and disordered proteins with molecular simulations and NMR spectroscopy” Roivant Sciences, New York, NY, (2021)
15. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” IDP Seminars, Virtual Seminar Series, IDPseminars.com, (2020)
16. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” Dewpoint Therapeutics, Boston, MA, (2020)

(Prior to Dartmouth)

17. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” University College of London, Thomas Young Centre Seminar Series, London, UK, (2019)
18. Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” University of Cambridge, Centre for Misfolding Diseases, Cambridge, UK, (2019)
19. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins” Institute for Research in Biomedicine, Chemistry & Structural Biology, Barcelona, Spain, (2019)

20. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”
    Sanofi R&D, Paris, France, (2019)
21. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”
    Institut Pasteur, Department of Structural Biology and Chemistry, Paris, France, (2019)
22. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”
    ETH Zürich, Department of Chemistry and Applied Bioscience, Zurich, Switzerland, (2019)
23. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”
    University of Copenhagen, Department of Biology, Copenhagen, Denmark, (2019)
24. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”
    Memorial Sloan Kettering Cancer Center, New York, NY, USA (2019)
25. “Molecular Recognition Mechanisms of Intrinsically Disordered Proteins”
    CUNY ASRC/City College of New York, Biochemistry, Biophysics & Biodesign Seminar Series, New York, NY, USA (2019)

Teaching Experience

- **Dartmouth College, General Chemistry. II (CHEM.006)**
  Lecture & Laboratory
  Topics: Quantum Mechanics, Bonding, Kinetics, Equilibria & Electrochemistry
- **Dartmouth College, Honors General Chemistry (CHEM.010)**
  Lecture & Laboratory
  Topics: Quantum Mechanics, Bonding, Thermodynamics, Kinetics, Equilibria & Electrochemistry
- **Dartmouth College, Physical Chemistry II (CHEM.076)**
  Lecture & Laboratory
  Topics: Quantum Mechanics, Molecular Spectroscopy, Kinetics, & Statistical Thermodynamics
- **Dartmouth College, Computational Methods in Chemistry & Biophysics (CHEM.101.6)**
  Project-based graduate course taught through a jupyter notebook / google collab interface.
  Topics: Statistical thermodynamics, molecular dynamics simulations, protein dynamics, protein folding, & enhanced sampling methods
  Course Materials: https://github.com/paulrobustelli/CHEM101.6
- **Dartmouth College, Graduate Research Colloquium in Computational & Theoretical Chemistry (CHEM.265)**
  Discussion of papers from the theoretical and computational chemistry literature
- **Columbia University, Advanced Biophysical Chemistry (Guest Instructor)**
  -Lectures and Computational Exercises on Protein Structure and Dynamics from NMR Spectroscopy and Theory and Applications of Molecular Dynamics Simulations.
- **New York Structural Biology Center / City College of New York, Graduate Protein NMR Spectroscopy (Guest Instructor)**
  - Special Topics Lectures: “Protein Structure and Dynamics from NMR Chemical Shifts”
- **New York Academy of Sciences Afterschool Science, Technology, Engineering, and Mathematics Mentoring Program**
  - 12-lesson mathematics and science outreach curriculum to a 6th grade class ‘

Mentoring Experience

- **Dartmouth College**
  Postdoctoral Scholars

- Jaya Krishna Koneru (2022 - Present), Korey Reid (2022 – Present), Aparajita Chakrabory (2022-Present), Emmanuele Scalone (2023- Present)

PhD Students

- Jiaqi Zhu (2019 - Present), Kaushik Borthakur (2020 - Present), Thomas Sisk (2021 - Present), Michelle Garcia (2022 – Present), Natalie Loui (2023-Present)

Undergraduate Students

- Vaishnavi Katragadda (Honors Senior Thesis Student - 2021-Present, Anjali Dhar (Honors Senior Thesis Student -2023-Present), Forrest Veilleux (2023-2024), Franklin Ruan (2022), Vaani Gupta (2021), Maeen Arslan (2021) Sarah Chong (2020)

Selected Awards and Honors

- Cottrell Scholar Award
  2024 – Invited Speaker, *Intrinsically Disordered Proteins Gordon Conference*, Les Diablerets, Switzerland
- 2024 – Invited Speaker, *Protein Folding Dynamics Gordon Conference*, Galveston, TX
- 2023 – Invited Speaker, *American Chemical Society Meeting Fall 2023*, San Francisco, CA
- 2023 – Invited Speaker, *Aqueous Supramolecular Chemistry Workshop*, Bozeman, MT
- 2023 – Invited Speaker & Discussion Leader, *Computational Aspects of Biomolecular NMR Gordon Conference*, West Dover, VT
- 2023 – Invited Speaker, *Prague Protein Spring Meeting*, Prague, Czech Republic
- 2022 – Invited Speaker, *Understanding the Role of Intrinsically Disordered Proteins in Cancer Biology*, *National Cancer Institute Workshop,* MD, USA
- 2022 – Dartmouth Innovations Accelerator for Cancer Development Award ($150,000 of research funding awarded by an external review panel of judges from venture capital firms and biotech companies)
- 2022 – Member, Dartmouth Cancer Center
- 2021 – Dartmouth Innovations Accelerator for Cancer Stu Trembly Award ($25,000 of research funding awarded by an external review panel of judges from venture capital firms and biotech companies)
- 2021 - Invited Speaker, *Intrinsically Disordered Proteins: Telluride Science Research Center Workshop*, CO, USA
- 2021 - Open Science Fellowship, Roivant Sciences
- 2020 - Member of Scientific Advisory Board & Scientific Consultant, Dewpoint Therapeutics
- 2020 - Member, Department of Biochemistry and Cell Biology, Dartmouth College, Hanover, NH
- 2020 - Member, Neukom Academic Cluster in Computational Science, Dartmouth College, Hanover, NH
- 2019 - Invited Speaker, *Biomolecules and Nanostructures*, Pomlewo, Poland
- 2019 - Invited Speaker, *Computational Biophysics at the Molecular and Mesoscales*, Quy Nhon, Vietnam
- 2019 - Member, Editorial Board, *Frontiers in Molecular Biosciences*
- 2017 - Invited Speaker, *CECAM Workshop: Disordered Protein Segments*, Paris, France
- 2010-2012 - NSF Postdoctoral Research Fellowship
- 2009-2010 - NSF Graduate Research Fellowship
- 2006-2009 - Gates Cambridge Scholarship
- 2006 - Member, Phi Beta Kappa
- 2005 - Barry M. Goldwater Scholarship
- 2005 - Member, Sigma Xi
- 2005 - Arnold and Mabel Beckman Scholarship
- 2005 - Achievement Rewards for College Scientists Foundation Scholarship (2005)

Professional Service

- Reviewer For: *Nature, Nature Methods*, *Nature Communications, Science Advances, Elife, Journal of the American Chemical Society, Proceedings of the National Academy of Sciences, Chemical Science, Nature Reviews Drug Discovery, Journal of Chemical Theory and Computation, Journal of Chemical Physics, Communications Chemistry, PLoS Computational Biology, Biochemistry*, *Biophysical Journal*,

Structure, *Journal of Physical Chemistry B, Communications Biology, Journal of Chemical Information and Modeling, Physical Chemistry Chemical Physics, Proteins: Structure, Function, and Bioinformatics, Journal of Biomolecular NMR, Life, Frontiers in Molecular Biosciences,*

- Professional Memberships: Protein Society, Biophysical Society, American Chemical Society
- Reviewer for Swiss National Super Computing Centre (CSCS) Grants, Swiss National Science Foundation Grants
- Dartmouth Committees: Graduate Student Entrance Committee (2020-2024, Chair 2021), Committee for Diversity, Inclusion, and Equity (2022-2024, Chair 2022-2023), Committee for Undergraduate Advising (2022-2024), Committee for Graduate Student Advising (2021-2022)
- Faculty Liaison for Dartmouth Chemistry Graduate Student Committee (2021-2024)