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Darian T. Yang
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https://darianyang.github.io/

Education:

PhD, Biophysics (GPA: 3.9)   August 2019 – August 2024
  Advisors: Lillian T. Chong PhD & Angela M. Gronenborn PhD
  University of Pittsburgh and Carnegie Mellon University
  Relevant Coursework*:* Statistical Mechanics, Statistical Computing,
  Machine Learning, Neural Networks & Deep Learning in Science
  Thesis: Invisible Protein States and How to View Them: Integrating ^{19}F NMR and Molecular Simulations

BS, Chemistry   August 2014 – May 2018
  University of Delaware, Newark, DE

Honors and Awards:

HPC Wire Award: Best use of HPC in Life Sciences	November 2025
DESRES Doctoral Fellowship	April 2024
A&S Grad Expo: Outstanding Presentation Award	March 2023
Andrew W. Mellon Predoctoral Fellowship	September 2022 – 2023
NSF: GRFP: Honorable Mention	March 2021
NIH: T32 Predoctoral Fellowship	August 2020 – 2021
Eurofins Impact Award	March 2019
Merck Index Award	May 2018

Research Experience:

Postdoctoral Research Fellow, University of Copenhagen   November 2024 – Present
Copenhagen, Denmark | Advisor: Kresten Lindorff-Larsen PhD

- Developing an adaptive sampling method with dynamic reweighting based on NMR relaxation rates.
- Integrating deep-learning methods with time-resolved experimental data and molecular simulations to sample protein-ligand (un)binding pathway intermediates.

Graduate Researcher, University of Pittsburgh   August 2019 – August 2024
Pittsburgh, PA | Advisors: Lillian T. Chong PhD & Angela M. Gronenborn PhD

- Derived force field parameters for integrating MD simulations with ^{19}F NMR.
- Used path sampling simulations and NMR experiments to study protein conformational dynamics.
- Developed and maintained software for weighted ensemble simulation and data visualization/analysis.
- Developed a reinforcement learning-based method for "binless" weighted ensemble simulations.

Research Assistant, University of Pittsburgh   July 2019 – October 2019
Pittsburgh, PA | Advisor: Andrew P. Hinck PhD

- Protein purification and backbone resonance assignment of an engineered TGF-β-mini-monomer.
- Optimization of an ^{13}C-^{1}H HSQC fragment-based ligand screening platform.

Scientist I, Merck Research Labs (Eurofins PSS)   June 2018 – June 2019
West Point, PA

- Process and automation development for a pneumococcal conjugate vaccine product.
- Advancement of downstream process parameters, conjugation conditions, and HPLC/LS methodology.
- Developed a Wyatt ASTRA® data pipeline used across vaccine research and commercialization.

Select Conferences:
- **Speaker:** The Danish Advanced Molecular Simulation Workshop – *Aaruhs, Denmark*; December 2025
- **Poster:** The 69th Benzon Symposium on Protein Design – *Copenhagen, Denmark*; September 2025
- **Lindau Scholar*:** The 74th Lindau Nobel Laureate Meeting in Chemistry – *Lindau, Germany*; July 2025
- **Poster*:** The Protein Society Annual Symposium – *Vancouver, Canada*; July 2024
- **Speaker:** MBSB Symposium – *Pittsburgh, PA*; May 2024
- **Speaker and poster:** PCHPI Symposium – *Pittsburgh, PA*; May 2024
- **Speaker and poster:** DESRES Doctoral Fellowship – *New York, NY*; April 2024
- **Poster:** OpenEye Scientific CUP XXIII – *Santa Fe, NM*; March 2024
- **Poster*:** The Biophysical Society Annual Meeting – *Philadelphia, PA*; February 2024
- **Discussion leader and poster award*:** GRC: Protein Folding Dynamics – *Galveston, TX*; January 2024
- **Speaker and poster*:** EBSA Congress & Summer Biophysics School – *Stockholm, Sweden*; August 2023
- **Speaker*:** Frontiers of Biophysics Summer Course – *Erice, Italy*; July 2023
- **Poster:** National Institutes of Health HIV Structural Biology Meeting – *Bethesda, MD*; June 2023
- **Poster*:** MolSSI: Machine Learning and Chemistry Workshop – *College Park*, *MD*; May 2023
- **Platform talk*:** The Biophysical Society Annual Meeting – *San Diego, CA*; February 2023
- **Speaker and poster**:** GRC: Protein Folding Dynamics – *Ventura, CA*; October 2022

* Awarded travel award or bursary

Publications:
- AT Bogetti, **DT Yang**, HE Piston, DN LeBard, LT Chong. "Lessons Learned from a Ligand-Unbinding Stress Test for Weighted Ensemble Simulations", *ACS Omega,* **2025***.*
- **DT Yang**, LT Chong, AM Gronenborn. "Illuminating an Invisible State of the HIV-1 Capsid Protein CTD Dimer using ^{19}F NMR and Weighted Ensemble Simulations"**,** *Proc. Natl. Acad. Sci.* **2025.**
- **DT Yang**, AM Goldberg, LT Chong. "Rare-Event Sampling using a Reinforcement Learning-Based Weighted Ensemble Method", *bioRxiv*, **2024**.
- **DT Yang**, LT Chong. "WEDAP: A Python Package for Streamlined Plotting of Molecular Simulation Data", *J. Chem. Inf. Model.,* **2024**.
- AJ Guseman, JJ González, **DT Yang**, AM Gronenborn. "Cumulative Asparagine to Aspartate Deamidation Fails to Perturb γD-Crystallin Structure and Stability", *Protein Science,* **2024**.
- AJ Guseman, LJ Rennick, S Nambulli, CN Roy, DR Martinez, **DT Yang**, F Binderwhala, S Veragara, RS Baric, Z Ambrose, WP Duprex, AM Gronenborn. "Targeting Spike Glycans to Inhibit SARS-CoV2 Viral Entry", *Proc. Natl. Acad. Sci.* **2023**.
- W Zhu, **DT Yang**, AM Gronenborn. "Ligand-capped Cobalt(II) Multiplies the Value of the Double-Histidine Motif for PCS NMR Studies", *J. Am. Chem. Soc.* **2023**.
- **DT Yang**, AM Gronenborn, LT Chong. "Development and Validation of Fluorinated, Aromatic Amino Acid Parameters for Use with the AMBER ff15ipq Protein Force Field", *J. Phys. Chem A,* **2022**.
- AT Bogetti, HE Piston, JMG Leung, CC Cabalteja, **DT Yang**, AJ DeGrave, KT Debiec, DS Cerutti, DA Case, WS Horne, and LT Chong. "A twist in the road less traveled: The AMBER ff15ipq-m force field for protein mimetics.", *J. Chem. Phys.* **2020**.

Manuscripts in Preparation:
- **DT Yang**, AT Bogetti, LT Chong. "Exploring the Role of an Allosteric Loop: Ligand Unbinding from the Kinesin Eg5 Motor Protein".
- **DT Yang**, S Palit, LT Chong, SK Saxena. "Integrating EPR and Weighted Ensemble Simulations to Characterize Dynamic Conformations of the LAO-binding Protein".

Mentorship:
- **January 2024 – March 2026:** Graduate student (collaborator)
  - Integrating weighted ensemble and electron paramagnetic resonance.
- **January – September 2024:** Graduate student
  - Integrating weighted ensemble and reinforcement learning.
- **September 2023:** Rotation student – Pairing weighted ensemble and least counts adaptive sampling.
- **September 2022:** Rotation students – MD data analysis using machine learning.
- **May – August 2022:** Summer Undergraduate Research Program (SURP) Student:
  - ^{19}F PCS calibration software, MD simulation and ^{19}F NMR for CypA and cyclosporin binding.

Teaching Experience:
- **Fall 2021:** teaching assistant for undergraduate course in quantum mechanics.
  - Guest lecture on quantum mechanics of NMR and force field development for MD.
- **Winter 2018:** Laboratory and lecture teaching assistant for undergraduate biochemistry.
  - Created grading rubrics and protocols, designed change in enzyme kinetics experiment.
- **Fall 2017-Spring 2018:** Lead weekly biochemistry workshop discussions.
- **Spring 2017:** Laboratory teaching assistant for an undergraduate microbiology course.

Science Outreach:

PittBio Outreach: Gene Team   July 2020, 2021
- Mentorship of high school students on a summer research project and general college preparation.
- 2020 Project(s): Automatic lab notebook generator, computational cancer risk estimator.
- 2021 Project(s): Drug discovery towards Alzheimer's disease using virtual screening.

Upward Bound Math & Science (UBMS)   December 2020, 2021
- Invited to give a career talk to UBMS high school students in southern Delaware.
- UBMS is a federally funded initiative to help socioeconomically disadvantaged and first-generation students prepare for and pursue a STEM focused career.
- Organized and taught a Python programming workshop during the Saturday Academy program.

Journal Club at Merck   September 2018 – June 2019
- Founding and leading a journal club with literature concerning vaccine process development.

Community Night at The Franklin Institute   August 2018 – June 2019
- Setting up and hosting a Merck sponsored hands-on science activity, engaging with children and families while fostering an interest in STEM through challenges and problem solving.
- Free admission to help open doors to Philadelphia's underserved communities.