Eric Anthony Chen

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RESEARCH INTERESTS

ML/AI computational chemistry, diffusion generative models, structure-based drug design

EDUCATION

New York University — **New York, NY**
Ph.D. in Chemistry — *May 2023–Aug 2025*
M.S. in Chemistry; GPA: 3.81 — *Sep 2019–May 2023*

Tufts University — **Medford, MA**
B.S. in Biochemistry; GPA: 3.75 — *Sep 2015–May 2019*

EXPERIENCE

Recurse Center — **New York, NY**
Participant — *Sep 2025–Present*

- Collaborate and develop a ML training and evaluation workflow for the prediction of protein engineering properties using protein language models and the AlignBio 2023 competition datasets

New York University - Department of Chemistry — **New York, NY**
Yingkai Zhang Lab — *Jan 2020–Aug 2025*

- Perform model fine-tuning and benchmarking on a curated database and increase the success rate of molecular generative models to predict allosteric ligand poses to the kinome by 34%
- Establish data-driven, ML workflow and toolkit to analyze protein–ligand conformational heterogeneity and assess prospective docking applications of allosteric compounds
- Collaborate across cross-functional teams with experimentalist to determine the binding location of a hit and with a software engineer to design robust training procedures and strategies
- Perform ensemble docking, molecular dynamics and free energy calculations to guide experimental direction of binding site determination of hit compound
- Developed reproducible code and workflows with documentation and tutorials, using best practices with Git, testing, and containerization on an HPC cluster

Tufts University - Department of Chemistry — **Medford, MA**
Yu-Shan Lin Lab — Aug 2017–May *2019*

- Utilize Bias-Exchange metadynamics for enhanced sampling of peptide macrocycles conformations
- *De novo* structure-based drug design of peptide macrocycle–collagen interactions by characterizing structural ensembles

Rutgers University-Camden - Center for Computational and Integrative Biology — **Camden, NJ**
Simeon Kotchoni Lab — *Jun 2018–Aug 2018*

- Development of protocol to analyze of pavement cell morphology in *A. thaliana* across mutants
- Use CellProfiler and Ilastik to process NeoScope SEM images
- Coding mathematical analyses of cell shape in R

PUBLICATIONS

2025 **Chen, E. A.,** Green, J. & Zhang, Y., Tuning DiffDock for Allosteric Structure-Based Drug Design to the Kinome. *In writing*

2025 **Chen, E. A.,** & Zhang, Y., Can Deep Learning Blind Docking Methods be used to Predict Allosteric Compounds? *J. Chem. Inf. Model.* **65** (7), 3737–3748 (2025)

2024 Soper, N.*, Yardumian, I.*, **Chen, E. A.***, Yang C., Ciervo S., Oom A., Desvignes L., Zhang, Y., & Lupoli, T. A repurposed drug interferes with nucleic acid to inhibit the dual activities of coronavirus Nsp13. *ACS Chem. Biol*. **19** (7), 1593-1603 (2024)

2023 Xia, S.*, **Chen, E. A.*** & Zhang, Y. Integrated Molecular Modeling and Machine Learning for Drug Design. *J. Chem. Theory Comput.* **19**, 21, 7478–7495 (2023)

2022 Yang, C., **Chen, E. A.** & Zhang, Y. Protein–Ligand Docking in the Machine-Learning Era. *Molecules* **27**, 4568 (2022).

2019 **Chen, E. A**. & Lin, Y.-S. Using synthetic peptides and recombinant collagen to understand DDR–collagen interactions. *Biochim. Biophys. Acta - Mol. Cell Res.* **1866**, 118458 (2019).

SCHOLARSHIPS/AWARDS/PRESENTATIONS

2025 DEI/Outreach Student Organizer Award
2025 AI4Chemistry Summit: Poster
2025 Computer Aided Drug Design – Gordon Research Conference: Poster
2025 Computer Aided Drug Design – Gordon Research Seminar: Poster and Invited Talk
2024 MoML 2024 Conference – Montreal: Poster
2023 ACS Fall – San Francisco: Poster
2022–2023 Simons Center Graduate Fellowship
2019 MacCracken Fellowship
2019 ACS Division of Organic Chemistry Outstanding, Senior Organic Chemistry Student
2019 Frederick S. Gimble and Amy L. Davidson Scholarship in Chemistry
2018 Tufts University Summer Scholars Program
2017 National Science Foundation, Research Experience for Undergraduates Scholarship at Rutgers University-Camden

TECHNICAL SKILLS

Programming Languages: Python, Bash, Distributed Systems, C++, Fortran, R
Programs: High-Performance Computing, SLURM system, Singularity containerization, PopSQL, Jupyter, PyTorch, PyTorch Lightning, NumPy, SciPy, Pandas, GitHub, Git, Wandb
Computational Chemistry Programs: RDKit, OpenBabel, Vina, Smina, DiffDock, AlphaFold2/3, Boltz-2, Amber, MM-PB/GBSA, GROMACS, PLUMED plugin, ChimeraX, Gaussian

DEI & OUTREACH/LEADERSHIP

Gotham Data Clinic **New York, NY**
Volunteer Program Assistant ***A**ug 2025–Present*
- Assist development of a new non-profit through programming and event planning

New York University; Chemistry Department **New York, NY**
DEI/Outreach Working Group Co-chair *Sep 2021–May 2025*
- Develop and execute the first strategic plan over 3 years to expand outreach efforts to enhance community engagement and diversity initiatives.
- Initiate and serve as the primary liaison for underserved NYC high school
- Lead group of 10–15 graduate students, faculty, and administrators to design chemistry outreach programming, oversee budget and impact assessment
- Organize and manage an annually run program that brings together up to 40 students and 80 volunteers for hands-on chemistry demonstrations, lunch, and building tours
- Recipient of the 2025 DEI/Outreach Student Organizer Award

FOCUS Mentorship Program **New York, NY**
Volunteer Mentor *Sep 2021–May 2023*
- Mentor first-year, first-generation POC undergraduates to facilitate college transition by building confidence, introducing resources, and encouraging community and academic success.

Gardner Pilot Academy Community School **Allston, MA**
Middle School Enrichment Teacher *Jun 2019–Aug 2019*

- Create and lead daily science, cultural, arts and sports programming aligned with Massachusetts state standards for summer school students
- Support staff to create positive environment for student development

Tufts Ultimate Frisbee Team **Medford, MA**
Captain: *Se*p 2017–*May* 2019; *A Team*: *Sep* 2015–*May* 2019*; Callahan Nominee*
- Logistical, organizational, strategic and financial responsibilities of a nationally competitive team and coaching staff

TEACHING

New York University **New York, NY**
Undergraduate Adjunct Instructor: *2020–2022*
- Chemistry 1/2/ Modern Chemistry lab; Chemistry 2/Computational Chemistry recitation

Tufts Literacy Corps **Medford, MA**
6th grade *Math Tutor* *Sep 2016–May 2017*
- Tutor and assist 3 students in 1-on-1 sessions with homework

Excel Learning Center **Brooklyn, NY**
7th grade/SHSAT Math Teacher *Jun 2016–Aug 2016*
Teaching Assistant *Jun 2015–Aug 2015*
- Prepare coursework and teach classrooms of 12–15 students