Alexander Matthew Payne

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EDUCATION

Tri-Institute (Weill Cornell, Sloan Kettering Institute, Rockefeller University) — New York, NY
Ph.D. in Chemical Biology — 2019 – 2025

University of North Carolina at Chapel Hill — Chapel Hill, NC
Biology (B.S) & Chemistry (B.A.), GPA 3.81 — 2014 – 2018

RESEARCH EXPERIENCE

Sloan Kettering Institute — New York, NY
Research Scholar in the Lab of Dr. John Chodera — Dec 2025 – Present

Sloan Kettering Institute — New York, NY
Graduate Student in the Labs of Dr. John Chodera and Dr. Richard Hite — May 2020 – Dec 2025

Open Science Drug Discovery for the Prevention of Future Pandemics

- Developed Python-based docking (drugforge) and analysis (harbor) pipelines with an international computational chemistry team using OpenEye and RDKit to evaluate strategies for docking molecules to the COVID Moonshot Initiative dataset of SARS-CoV-2 Main Protease ligands

Modeling Parkinson's Disease-linked Mutations in TMEM175

- Built improved TMEM175 protein models incorporating cryo-EM data and performed molecular dynamics simulations using OpenMM to investigate Parkinson's disease-linked mutations (M393T, Q65P)

Architecture and activation of single-pass transmembrane receptor guanylyl cyclase

- Collected and re-analyzed cryo-EM data to resolve full-length GC-A structure at <8 Å resolution, overcoming previous limitations that only captured the extracellular domain, contributing to a publication

Weill Cornell Medicine — New York, NY
Rotation Student in the Lab of Dr. Harel Weinstein — Jul 2019 – Sep 2019

Computational Probing of Structural Determinants for Deficient Rhodopsin Dimerization in Retinitis Pigmentosa

- Analyzed coarse-grained simulations of Rhodopsin mutations, determining differences in dimerization

UNC Department of Medicine — Chapel Hill, NC
Research Assistant in the Lab of Dr. Brian Kuhlman — 2017 – 2019

Structure Guided Design of Zika and Dengue Virus Subunit Vaccine Antigen

- Designed Dengue Virus Envelope protein mutants with improved homodimer stability using Rosetta Design and tested their affinity for neutralizing antibodies with mammalian display flow cytometry

WORK EXPERIENCE

Schrödinger, Inc. — New York, NY
Desmond Life Science Software Team Intern — Summer 2023

- Benchmarked performance of CHARMM36m, OPLS2005, OPLS4, and L-OPLS forcefields on membrane bilayers including POPC, POPE, DMPC, and DPPC
- Established P2Y1R, a GPCR, as a benchmark FEP+ dataset to test the ability of FEP+ to predict ligand affinities for an active site that is membrane-facing

- Interfaced with Schrödinger's forcefield, drug discovery, and application scientist teams to disseminate findings and guide future research

SKILLS AND CERTIFICATIONS

Residential School on Medicinal Chemistry and Biology in Drug Discovery – Drew University, June 2024

Introduction to Modeling in Drug Discovery – Schrödinger, Nov 2021

Python 3 Course – Codecademy, Apr 2019

Molecular Modeling

PyMOL · ChimeraX · OpenEye · OpenMM · OpenFE · Folding@home · CHARMM-GUI · Glide · Maestro · FEP+

Programming

Python · Jupyter · GitHub (actions · CI · projects) · bash · LSF · SLURM · NextFlow

TEACHING EXPERIENCE

The City College of New York New York, NY
Adjunct Assistant Professor, Biophysics in Applications (PHYS 42300) Aug 2025 – Dec 2025

- Prepared and taught lectures for a class of 24 students on the basics of biophysics and and its applications in drug discovery and protein design

Weill Cornell Medicine New York, NY
Teaching Assistant, Core Principles of Molecular Biophysics Jan 2021 – July 2021, Jan 2022 – July 2022

SELECTED PUBLICATIONS

Payne, A. M., et. al. How many crystal structures do you need to trust your docking results? bioRxiv September 24, 2025, p 2025.09.19.677428. https://doi.org/10.1101/2025.09.19.677428.

Castellanos, M. A., **Payne, A. M.**, et. al. A Structure-Based Computational Pipeline for Broad-Spectrum Antiviral Discovery. bioRxiv July 30, 2025, p 2025.07.29.667267. https://doi.org/10.1101/2025.07.29.667267.

MacDermott-Opeskin, H., (...), **Payne, A. M.**, (...). A Computational Community Blind Challenge on Pan-Coronavirus Drug Discovery Data. ChemRxiv August 26, 2025. https://doi.org/10.26434/chemrxiv-2025-zd9mr-v2

Boby, M. L., (...), **Payne, A. M.**, (...). Open Science Discovery of Potent Noncovalent SARS-CoV-2 Main Protease Inhibitors. Science 2023, 382 (6671), eabo7201. https://doi.org/10.1126/science.abo7201.

Kudlacek, S. T., Metz S., Thiono D., **Payne, A. M.**, (. . .), Kuhlman, B. Designed, highly expressing, thermostable dengue virus 2 envelope protein dimers elicit quaternary epitope antibodies. Science Advances (2021). DOI: 10.1126/sciadv.abg4084

Croll, T. I., (. . .), **Payne A. M.**, (. . .), Thorn. A. Making the invisible enemy visible. Nat Struct Mol Biol 28, 404–408 (2021). DOI: 10.1038/s41594-021-00593-7

Khelashvili, G., (. . .), **Payne, A. M.**, (. . .) Menon, A. K. Unusual mode of dimerization of retinitis pigmentosa-associated F220C rhodopsin. Sci Rep 11, 10536 (2021). DOI: 10.1038/s41598-021-90039-3

Kudlacek, S. T., (. . .), **Payne, A. M.**, (. . .), Kuhlman, B. Physiological temperatures reduce dimerization of dengue and Zika virus recombinant envelope proteins. Journal of Biological Chemistry 293, 8922–8933 (2018). DOI: 10.1074/jbc.RA118.002658

SELECTED POSTERS AND PRESENTATIONS

Computer Aided Drug Design Gordon Research Conference Portland, ME – 2025
Poster – How many crystal structures does it take to trust your docking results?

Free Energy Workshop Boston, MA – 2025
Poster – How many crystal structures does it take to trust your docking results?

OpenEye CUP Santa Fe, NM – 2025
Poster – Towards An Efficient Protocol for Accurately Triaging Molecules in the Development of a SARS-CoV-2 Main Protease Inhibitor

Gerard van Westen Group Seminar Leiden University, Leiden, NL – 2023
Invited Talk – Docking strategies in an information-rich environment

Folding@NYC Meeting New York, NY – 2023
Invited Talk – How Do Parkinson's Disease Causative and Protective TMEM175 Mutants Alter TMEM175's Thermodynamic Landscape?