

Alexander Matthew Payne

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[Google Scholar](#) | [GitHub](#) | [LinkedIn](#)

EDUCATION

2019-Present Ph.D., [Tri-Institutional Ph.D. Program in Chemical Biology](#), New York, NY

2014-2018 Biology (B.S.), Chemistry (B.A), University of North Carolina at Chapel Hill, GPA: 3.81

RESEARCH PROJECTS

2020-Present PhD Candidate, Chodera and Hite Labs, Sloan Kettering Institute, New York, NY

“ASAP: Open Science Drug Discovery for the Prevention of Future Pandemics”

- Contributed to the development of a python docking and analysis pipeline
 - [choderalab/covid-moonshot-ml](#): a to-be-renamed repository for ASAP Discovery computational chemistry efforts
- Explored methods of transferring knowledge of molecule activity to related viral targets
- Collaborated with an international team to triage molecules for the development of antiviral drugs

“Pursuing Allosteric Activators of an Ion Channel on the Road to a Parkinson's Disease Therapeutic”

- Built an improved protein model using ChimeraX, Coot, and Phenix, and set up simulations using CHARMM-GUI
- Ran simulations of the protein using OpenMM on [Folding@home](#) (F@h) and analyzed with MDTraj
- Maintained GitHub repositories of simulation setup and analysis
 - [choderalab/tmem175-allostery-analysis-CL](#): local simulations and analysis in preparation for F@h
 - [choderalab/fah-analysis-tmem175](#): analysis of F@h data using PyEMMA
 - [choderalab/enhanced-sampling-tmem175](#): setup and analysis of some enhanced sampling simulations

“Structural Analysis of a Dynamic Single-Pass Transmembrane Protein”, in collaboration with the Huang Lab at WCM

- Collected CryoEM data and extensively classified using Relion and CryoSPARC, with a paper submitted

2019 Rotation Student, Weinstein Lab, Weill Cornell Medical College, New York, NY

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

- Analyzed Martini simulations of Rhodopsin mutants using Tcl/Tk (a scripting language) and Python and visualized the results with VMD
- Determined differences in dimerization contacts between mutants, earning co-authorship in Khelashvilli 2021

2017-2019 Research Assistant, Kuhlman Lab, UNC Department of Medicine, Chapel Hill, NC

“Structure Guided Design of Zika and Dengue Virus Subunit Vaccine Antigen”

- Designed and tested Dengue Virus Envelope protein mutants with improved homodimer stability using Rosetta Design, resulting in co-authorship in Kudlacek 2018 and Kudlacek 2021
- Wrote XML, Python, and Bash scripts to run Rosetta on an HPC cluster and analyze the results

SKILLS AND CERTIFICATIONS

Intro to Molecular Modeling in Drug Discovery, Schrodinger (Online)

Learn Python 3, Codecademy (Online)

Structural Biology: CryoSPARC, Relion, Phenix, ChimeraX, Coot, Isolde, PyMOL

Molecular Simulation: OpenMM, Folding@home, CHARMM-GUI, GROMACS

Python Packages: openeye, mdtraj, mdanalysis, pyemma, pandas, numpy, plotly, matplotlib

Software Tools: Bash, GitHub, PyCharm, iTerm, LSF, Slurm

Organizational Tools: Slack, Notion, Microsoft Office Suite

ACTIVITIES AND EXPERIENCES

2022 Visiting Scientist (6 weeks), Delemotte Lab at SciLifeLab, Solna, Sweden

- Learned methods for running enhanced sampling molecular dynamics experiments on membrane proteins
- 2021, 2022** **Teaching Assistant**, “Core Principles of Molecular Biophysics”, Weill Cornell Medical College, New York, NY
- Facilitated discussion and learning in lectures and active learning sessions with 5-10 students
 - Graded Problem Sets, presentations, and introduced the ability to make corrections on previous Problem Sets
- 2021-Present** **Member**, Folding@home Scientific Communications Team
- 2020-Present** **Member**, Coronavirus Structural Biology Task Force, headed by Andrea Thorn
- 2019-Present** **Member**, Science Education and Policy Association, Weill Cornell Medical College, New York, NY
- 2017** **Committee Member**, March for Science, Sydney, Australia

PUBLICATIONS

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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1074/jbc.RA118.002658)

CONFERENCES & SEMINARS

- 2022** **Poster**, “Probing the mechanism of Parkinson’s Disease protective and causative TMEM175 mutations using Folding@home”, 2nd Annual COMPPÅ symposium, New York
- 2021** **Poster**, “Pursuing Allosteric Activators of TMEM175 on the Road to a Parkinson's Disease Therapeutic”, 17th Annual Tri-Institutional Chemical Biology Symposium
- 2022** **Departmental Seminar**, “Combining Cryo-EM and Molecular Dynamics to Describe Protein Conformational Landscapes”, Molecular Biophysics Training Program, Research-in-Progress Seminar
- 2019** **Poster**, “Computational Probing of Structural Determinants for Deficient Rhodopsin Dimerization in Retinitis Pigmentosa”, 15th Annual Tri-Institutional Chemical Biology Symposium

REFERENCES

- [John D. Chodera](#) Associate Member, Computational Biology Program, Sloan Kettering Institute
- [Richard K. Hite](#) Associate Member, Structural Biology Program, Sloan Kettering Institute
- WCM** Weill Cornell Medical College
- TPCB** Tri-Institution Ph.D. Program in Chemical Biology, including SKI, WCM, and Rockefeller University
- SKI** Sloan Kettering Institute