**Alexander Matthew Payne**

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[Google Scholar](https://scholar.google.com/citations?user=uXUBXMAAAAAJ&hl=en) | [GitHub](https://github.com/apayne97) | [LinkedIn](https://www.linkedin.com/in/alexander-matthew-payne-0899a0a1/)

**EDUCATION**

**­­­­­­­­­­­­­­­­­­­2019-Present Ph.D.,** [Tri-Institutional Ph.D. Program in Chemical Biology](https://chembio.triiprograms.org/), 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](https://github.com/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](https://foldingathome.org/) (F@h) and analyzed with MDTraj
* Maintained GitHub repositories of simulation setup and analysis
  + [choderalab/tmem175-allostery-analysis-CL](https://github.com/choderalab/tmem175-allostery-analysis-CL): local simulations and analysis in preparation for F@h
  + [choderalab/fah-analysis-tmem175](https://github.com/choderalab/fah-analysis-tmem175): analysis of F@h data using PyEMMA
  + [choderalab/enhanced-sampling-tmem175](https://github.com/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**](https://www.choderalab.org/)Associate Member, Computational Biology Program, Sloan Kettering Institute

[**Richard K. Hite**](https://www.mskcc.org/research/ski/labs/richard-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