

# AYUSH DEEP

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## EDUCATION

### Memorial Sloan Kettering Cancer Center

PhD in Cancer Biology

Advisors: Prof. John Chodera and Prof. Caleb Lareau

New York, NY

Jul 2024 - Present

### Eidgenössische Technische Hochschule Zürich

M.Sc. in Molecular and Structural Biology

Thesis title: *Molecular Dynamics Simulations of Darobactin Analogues*

Advisor: Prof. Sereina Riniker

Zürich, CH

Sept 2021 - Nov 2023

### Albany College of Pharmacy and Health Sciences

B.Sc. in Pharmaceutical Science, minor in Mathematics

Thesis title: *Overexpression and Purification of Human mtEF4*

Advisor: Prof. Rajendra K. Agrawal

Albany, NY

Aug 2015 - May 2019

## RESEARCH EXPERIENCE

### Chodera Lab and Lareau Lab, MSKCC

PhD Student

New York, NY

Aug 2025 - Present

- Applied Molecular dynamics simulations simulations in openMM and free energy calculations in PERSES to understand the effects of mutations in cancer relevant kinases
- Redesigned membrane proteins to express in a soluble manner with the same folds using protein design tools using ProteinMPNN
- Designed minibinders to target specific protein and non-protein cancer antigens using Bindcraft, Boltz-Design, and Bindcraft

### Dar Lab and Lima Lab, MSKCC

Rotation Student

New York, NY

March 2025 - June 2025

- Utilized cofolding models to predict small-molecule-protein interactions
- Use analytical size exclusion chromatography to validate interactions enriched in mass spectrometry data and cofolding predictions
- Conducted confocal microscopy to explore effects of small molecules on nuclear localization of particular kinases

### Zhao Lab, MSKCC

Rotation Student

New York, NY

January 2025

- Utilized large scale computational cofolding screens to identify potential interactors of the SMC5/6 complex
- Utilized all atom cofolding models to predict nucleotide-protein interactions which were further validated with yeast genetic screens

### Riniker Lab, ETH Zürich

Masters Thesis Student

Zürich, CH

April 2023 - Nov 2023

- Utilized AMBER and GROMACS softwares to perform Molecular Dynamics simulations, exploring the interactions between macrocyclic peptides and membrane proteins
- Analyzed the properties of candidate novel macrocyclic compounds using Python and cpptraj for structure-function analysis
- Used cheminformatics toolkits such as RDKit and OEChem for conformer generation of macrocyclic peptides

### Ban Lab, ETH Zürich

Semester Project Student

Zürich, CH

Oct 2022 - Jan 2023

- Investigated the role of proteins involved in non-canonical translation initiation by in-vitro translation techniques
- Standardized an immunodepletion protocol within an in-vitro translation system

**Jonas Lab, ETH Zürich**  
*Research Assistant*  
*Semester Project Student*

Zürich, CH  
Jun 2022 - Aug 2022  
Jan 2022 - Jun 2022

- Investigated the early steps of ribosome biogenesis by using biochemical techniques such as in-vitro transcription and northern blotting
- Gained experience in mammalian cell culture and transfection of human cell lines
- Conducted pulldown assays to determine interacting partners of protein complexes involved in early stages of ribosome biogenesis

**Agrawal Lab, Wadsworth Center**  
*Research Assistant*  
*Undergraduate Student Researcher*

Albany, NY  
Jun 2019 - May 2021  
Jun 2017 - May 2019

- Over-expressed mammalian translation factors of interest in bacterial systems. Purified these proteins using FPLC and a variety of chromatography methods (His-tag, ion exchange, GST-tag, size exclusion)
- Designed and standardized a GTPase assay to assess the difference in antibiotic effectiveness between bacterial and mitochondrial translational factors
- Processed single particle cryo-EM data using cryoSPARC and RELION.
- Used CHARMM molecular dynamics package to simulate antibiotic binding to the ribosome
- Trained in the process of making high quality grids (carbon evaporation, vitrification) for cryo-EM
- Mentored high school interns in basic molecular biology techniques and protein purification

**Zheng Lab, ACPHS**  
*Undergraduate Student Researcher*

Albany, NY  
Oct 2015 - May 2017

- Wrote a script in Python for purposes of visualizing affinity of different cannabinoids to the CB1 and CB2 GPCR receptors in terms of binding affinity and agonistic, antagonistic, and inverse-agonistic properties.

**Genspace**  
*iGEM Student Member*

Brooklyn, NY  
Jun 2016 - Nov 2016

- Part of a team participating in the iGEM competition. Involved in the design and cloning of plasmid vectors into *E. coli*. Used RT-qPCR to quantify the plasmid copy number of one of the most commonly used plasmid backbones in the competition. This project resulted in the Genspace team winning a medal for Best Measurement project. Details of all projects can be found at <http://2016.igem.org/Team:Genspace>

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## PREPRINTS

1. Soneya Majumdar\*, **Ayush Deep\***, et al. The small mycobacterial ribosomal protein, bS22, modulates aminoglycoside accessibility to its 16S rRNA helix-44 binding site. bioRxiv (2023); <https://www.biorxiv.org/content/10.1101/2023.03.31.535098v1>

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## PUBLICATIONS

1. Ravi K. Koripella, **Ayush Deep**, Ekansh K. Agrawal, Pooja Keshavan, Nilesh K. Banavali, and Rajendra K. Agrawal. Distinct mechanisms of the human mitoribosome recycling and antibiotic resistance. Nat Commun 12, 3607 (2021); <https://doi.org/10.1038/s41467-021-23726-4>

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## POSTER PRESENTATIONS

1. Nathaniel Spaziani, **Ayush Deep**, Andrew Thurston, HaiAn Zheng. System Pharmacognosy Mapping of Phytocannabinoids for CB1/CB2 Activity and Specificity. International Cannabinoid Research Society Symposium. June 2017.

## EXTRACURRICULARS

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### Resonance Jams

*Volunteer and Board Member*

Zürich, CH

Jan 2022 - Jan 2024

- Volunteered as part of the music organization, Resonance, to organize weekly open jams for musicians in Zürich

## SKILLS

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Languages: English (native), Hindi (native), Spanish (A2)

Software: Python, PyTorch, Jupyter, Bash, L<sup>A</sup>T<sub>E</sub>X, OpenMM, Rosetta, GROMACS, PyMOL, Chimera/ChimeraX, COOT, cryoSPARC, RELION, PHENIX, Bindcraft, RFDiffusion, Boltz-design, RDKit, OEChem, Vim

## AWARDS

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### Student Biolab Ideathon 1st place

3,000 CHF bio-hackathon award for the design of better biodegradable polymers

ETHZ

Nov 2022

### Excellence Scholarship (ESOP)

36,000 CHF stipend and full tuition waiver for top 2% of entering Master's students

ETHZ

Sept 2021 - Dec 2022

### Dean's Scholarship

\$20,000 tuition deduction award for high GPA and standardized testing scores

ACPHS

Aug 2015 - May 2019

### Pharmaceutical Science Scholarship

\$5,000 tuition deduction award for high GPA and standardized testing scores

ACPHS

Aug 2015 - May 2019

### Dean's List

Recognized for GPA > 3.5

ACPHS

Fall 2015 - Spring 2017, Fall 2018, Spring 2019

### Best Measurement Project

Awarded to the best synthetic biology measurement project

iGEM

Nov 2016

## REFERENCES

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**Prof. John Chodera**

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