

# Pranav Ballaney

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## EDUCATION

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### Birla Institute of Technology and Science, Pilani

Goa, India

*Master of Science in Biological Sciences*

*August 2018 – July 2023 (expected)*

*Bachelor of Engineering in Computer Science*

**Cumulative GPA:** 9.24/10

### Delhi Public School, Indira Nagar

Lucknow, India

*All India Senior Secondary Certificate Examination*

*Graduated May 2017*

**Percentage in Class 12:** 89.4%

**CGPA in Class 10:** 10/10

## RESEARCH EXPERIENCE

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### Purdue University, USA

September 2022 – Present

*Research Intern at the Purdue Institute for Drug Discovery*

Currently working application of computational methods to drug design, under the supervision of Prof. Philip Low, Presidential Scholar for Drug Discovery. My research aims to design ligands through deep learning and structural modeling on Schrodinger software. I am also working on a mathematical model to guide the design of ligands for a bispecific-adaptor-mediated CAR T cell therapy.

### Western University, Canada

June 2022 – August 2022

*Visiting Research Student under the Mitacs Globalink Research Internship Program*

Performed molecular dynamics (MD) simulations to understand the mechanisms of extrusion of proteins from charged water droplets, under the supervision of Prof. Styliani Conostas, Department of Chemistry, Western University. Simulations were carried out using NAMD. An article is in preparation.

### Research Projects, BITS Goa, India

January 2021 – May 2022

*Supervised by Prof. Raviprasad Aduri*

- Performed molecular dynamics simulations using GROMACS for virtual screening of small-molecule inhibitors for the SARS-CoV-2 3CL protease.
- Worked on evaluation of computational tools used to predict RNA secondary structures. Article in preparation.

### National Resource for Network Biology

May 2021 – August 2021

*Student Developer under Google Summer of Code 2021*

[\(Link to Project\)](#)

Developed a simulator for mathematical models for systems biology in the Systems Biology Markup Language (SBML), along with parsers for SBML and MathML in Rust, under the guidance of Prof. Akira Funahashi. The simulator applies the Runge-Kutta and Runge-Kutta-Fehlberg methods for numerical integration of ODEs in an SBML model.

### CSIR - Institute of Genomics and Integrative Biology, India

February 2021 - July 2021

Developed Python software and a web server to generate structures of autophagosomes for molecular dynamics simulations and performed simulations to understand their formation, under the guidance of Dr. Lipi Thukral, Senior Scientist at the Computational Structural Biology lab.

### International Genetically Engineered Machine (iGEM) Competition

November 2019 – November 2020

*Software Team Lead, BITS Goa*

[\(Link to Project\)](#)

- Awarded the **Gold Medal** along with two Special Prizes for Best Software Tool and Best Composite Part
- Worked under the supervision of Dr. Sumit Biswas, as part of the first iGEM team from BITS Goa, on reduction of post-harvest losses of sugar in sugarcane, by using genetically engineered bacterial systems.

## PUBLICATIONS

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Mishra, B., Ballaney, P., Saha, G., Shinde, A., Banerjee, S., Thimmakondur, V. S., & Aduri, R. (2022).

**An *in-silico* discovery of potential 3CL protease inhibitors of SARS-CoV-2 based upon inactivation of the cysteine 145-Histidine 41 catalytic dyad.**

*Journal of Biomolecular Structure and Dynamics*, 1–20.

<https://doi.org/10.1080/07391102.2022.2047108>

## WORK EXPERIENCE

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### Debian

May 2020 – August 2020

*Student Developer under Google Summer of Code 2020*

*([Link to Project](#))*

- Worked on quality assurance and continuous integration of software in life sciences and medicine.
- Designed test suites for over 40 applications in bioinformatics, performed bug fixes and added several new packages to the Debian operating system.

## SCHOLARSHIPS AND AWARDS

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### Mitacs Globalink Research Internship Award

March 2022

Awarded to international students for carrying out a research internship at a public university in Canada.

### International Genetically Engineered Machine (iGEM) Competition 2020

November 2020

*Gold Medal and Special Prizes for Best Software Tool and Best Composite Part*

*([Link to Project](#))*

### Institute Merit-cum-need Scholarship, BITS Goa

August 2018 - Present

Awarded every semester to top 3% students to cover 80% of tuition fees.

## TECHNICAL SKILLS

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**Programming Languages:** Python, R, C, C++, Java, Rust, HTML, CSS, JavaScript, Bash

**Software frameworks:** Schrodinger suite, VMD, NAMD, GROMACS, MDAAnalysis, NumPy, Pandas

## RELEVANT COURSES

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**Biology:** Biochemistry, Microbiology, Cell and Molecular Biology, Bioinformatics, Genetics, Recombinant DNA Technology, Immunology, Biophysics, Developmental Biology, Biomolecular Modelling

**Mathematics:** Mathematics I (Multi-variable and Vector Calculus), Mathematics II (Linear Algebra and Complex Analysis), Mathematics III (Differential Equations), Probability and Statistics, Nonlinear Dynamics and Chaos

**Computer Science:** Object Oriented Programming, Data Structures and Algorithms, Database Management Systems, Operating Systems, Computer Architecture, Deep Learning, Compiler Construction, Design and Analysis of Algorithms, Computer Networks, Quantum Information and Computing

## OTHER EXPERIENCE

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- **Teaching Assistant for Computer Programming and Digital Design:** Responsibilities include conducting labs for students.
- **Student Mentor under the Academic Assistance Program for General Biology:** Responsibilities included conducting tutorials for first-year students.
- **Peer Mentor as a part of the Peer Mentorship Program:** Helping students navigate through college and looking after their academic and personal interests.