

Pranav Ballaney

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EDUCATION

Purdue University, USA

PhD Student at the Department of Chemistry

Goa, India

August 2023 – present

Birla Institute of Technology and Science, Pilani

Master of Science in Biological Sciences

Bachelor of Engineering in Computer Science

Cumulative GPA: 9.36/10

Goa, India

August 2018 – July 2023

RESEARCH EXPERIENCE

Purdue University, USA

Research Intern at the Purdue Institute for Drug Discovery

September 2022 – May 2023

Worked on computational drug design, under the supervision of Prof. Philip Low, Presidential Scholar for Drug Discovery. Designed ligands for cancer therapy through deep learning and structural modeling on Schrodinger software. Developed a mathematical model to guide the design of ligands for a bispecific-adaptor-mediated CAR T cell therapy.

Western University, Canada

Visiting Research Student under the Mitacs Globalink Research Internship Program

June 2022 – August 2022

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.

Research Projects, BITS Goa, India

Supervised by Prof. Raviprasad Aduri

January 2021 – May 2022

- 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

Student Developer under Google Summer of Code 2021

May 2021 – August 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

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.

February 2021 - July 2021

International Genetically Engineered Machine (iGEM) Competition

Software Team Lead, BITS Goa

November 2019 – November 2020

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

- 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

Kwan, V., Ballaney, P., Titiksha, Consta, S. (2023).

Limitations of Atomistic Molecular Dynamics to Reveal Ejection of Proteins from Charged Nanodroplets.

J. Phys. Chem. B, 2023, 127, 21, 4829–4842.

<https://doi.org/10.1021/acs.jpcc.3c01313>

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

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

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.

Summer Internship Assistance, Alumni Relations Cell, BITS Goa

May 2023

Awarded to BITS Goa students to support their summer internships.

Travel Support, International Programmes and Collaboration Division, BITS Goa

October 2022

Awarded to BITS Goa students working on their thesis at foreign universities.

TECHNICAL SKILLS

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

Software frameworks: Schrodinger suite, VMD, NAMD, GROMACS, MDAnalysis, NumPy, Pandas

RELEVANT COURSES

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

- **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.