Abhinav Mishra

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Computational Biologist • Bioinformatics • Scientific Software

Technical Skills

Languages	Python, R, C++, Bash/Shell, Nextflow DSL2, Perl
HPC / Parallel	SLURM (batch jobs), MPI (`mpi4py`), OpenMP, SIMD/AVX2 (C++), JAX (GPU-accelerated ODE/PDE)
Data / Workflows	Snakemake, Nextflow DSL2, Git/GitHub, PyPI packaging, Zenodo/DOI archiving
Scientific	ODE / stochastic modelling, Bayesian parameter estimation, nonlinear optimisation, sensitivity analysis, PBPK modelling, biostatistics
Bioinformatics	RNA-seq (bulk & single-cell), differential expression (DESeq2/GEO2R/TCGA), variant calling (GATK/samtools), phosphoproteomics, sequence alignment (NW/SW/LCS)
Tools	samtools, GATK, ggplot2, matplotlib, R/Shiny, Quarto, PyMol (basic)

Education

M.Sc. Bioinformatics, Freie Universität Berlin, Germany 2025

Thesis: Mathematical Optimization of Signalling Networks in Triple Negative Breast Cancer

B.Tech. Bioinformatics, Jaypee University of Information Technology, India 2017

Thesis: Identification of Potent Biomarkers for Prostate Cancer Through AR, MAPK, and mTOR Pathway Mining

Research Experience

Research Intern *Institute for Biology, Humboldt-Universität zu Berlin* Jan 2025–March 2025

- Developed a physiologically based pharmacokinetic (PBPK) model of Tirzepatide from clinical data, formulating multi-compartment ODE systems for absorption, distribution, and clearance dynamics.
- Automated model fitting and simulation in Python using reproducible workflow design; integrated cleanly with Dr. König's existing pharmacokinetic framework codebase. Focused on reproducible model fitting, simulation, and interpretation of clinical pharmacokinetic data.

Master Thesis Student *Theoretical Biophysics, Humboldt-Universität zu Berlin* May 2024–April 2025

- Built a complete optimization framework for reconstructing phosphorylation signalling networks in triple-negative breast cancer from time-resolved kinase–substrate datasets.
- Structured the framework (*PhosKinTime*) as a modular, documented Python package with versioned releases and a public documentation site, enabling reuse by collaborating research groups.

Bachelor Thesis Student *Jaypee University of Information Technology, India* Feb 2016–Mar 2017

- Implemented a biomarker discovery pipeline integrating GEO2R differential expression analysis, clustering in MeV, and R/Shiny visualization to explore AR/MAPK/mTOR pathways in prostate cancer.
- Identified potential biomarkers and network modules using pathway mining and statistical analysis.

Project Researcher *Jaypee University of Information Technology, India* Aug 2015–Mar 2016

- Designed a drug docking workflow combining Discovery Studio and Glide XP for virtual screening of small molecules against target proteins.
- Prepared structures, optimized docking protocols, and analyzed binding interactions to shortlist candidate compounds.

Conferences & Presentations

MATH+ Day Seminar, Berlin	2024
RECOMB	2020
R&D Expo IEEE–JUIT	2016
NSCSB	2016

Awards & Honours

3rd Prize (Poster), NSCSB, JUIT India	2016
GATE Qualified, AIR 681	2018

Languages

English (native), Hindi (native), German (basic A1/A2)

Career Timeline Notes

Personal health and family responsibilities	2018–2020
Entrance examination preparation (engineering)	2012–2013

Selected Software & Publications

1. **Mishra, A.** & König, M. (2025). *Multi-compartment PBPK model of Tirzepatide (GLP-1/GIP receptor agonist) calibrated from clinical time-course data; integrated with existing pharmacokinetic frameworks for reproducible simulation and sensitivity analysis (v0.9.3).*
   [DOI] | [Report]
   Python **ODE** **Zenodo** **Reproducible**
2. **Mishra, A.** (2025). *PhosCrosstalk: Global phospho-network ODE modelling framework; multi-objective optimisation over kinase–substrate interaction graphs, designed as a reusable, structured Python API for cross-lab use.*
   [GitHub]
   Python **ODE** **Optimisation** **Open Source**
3. **Mishra, A.** (2025). *PhosKinTime: Optimization-driven ODE modelling of phosphorylation signalling dynamics; modular Python package with non-linear least-squares and constrained optimisation backends, sensitivity analysis, and full documentation. Framework design is generalisable to transcription kinetics and gene regulatory network modelling.*
   [DOI] | [GitHub] | [Docs]
   Python **PyPI** **Zenodo** **Documented**
4. **Mishra, A.** (2025). *pynetphorest: Python re-implementation of the NetPhorest/NetworKIN kinase–substrate prediction framework; published to PyPI for community reuse.*

[DOI] | [PyPI]

Python **PyPI** **Zenodo** **Open Source**

5. **Mishra, A.** (2025). *CETSAx–NADPH: Snakemake workflow for rule-based, reproducible analysis of NADPH-driven protein thermal stability response data from CETSA proteomics experiments.*
   [GitHub] | [Docs]
   Snakemake **Bash** **Workflow** **Documented**
6. **Mishra, A.** (2025). *nf-illumina2lineage: Nextflow pipeline for end-to-end SARS-CoV-2 genome assembly and lineage assignment from Illumina reads; portable, documented, production-ready for multi-group deployment.*
   [DOI] | [GitHub]
   Nextflow **Bash** **Zenodo** **Linux**
7. **Mishra, A.** (2025). *GRmap: Snakemake pipeline for genome read mapping and annotation; parameterised rules enabling reproducible, cluster-ready runs.*
   [DOI] | [GitHub] | [Docs]
   Snakemake **Bash** **HPC** **Zenodo**
8. **Mishra, A.** (2025). *SequenceAligner: C++ implementation of LCS, Needleman–Wunsch, and Smith–Waterman algorithms; deployed with OpenMPI for distributed computation, Docker-containerised with FastAPI backend and React frontend.*
   [DOI] | [GitHub] | [Docs]
   C++ **MPI** **Docker** **REST API**
9. **Mishra, A.** (2025). *CasTuner (Python Port): kinetic modelling and ODE simulation toolkit for CRISPR-Cas regulatory systems; versioned release with full documentation.*
   [DOI] | [GitHub] | [Docs]
   Python **ODE** **Zenodo** **Documented**
10. **Mishra, A.** (2025). *Hsp90 smFRET Kinetic Modeling and Analysis Pipeline: automated analysis pipeline for single-molecule FRET data from Hsp90 conformational dynamics experiments.*
    [GitHub]
    Python **Pipeline** **Open Source**
11. Asati, N.; **Mishra, A.**; Shukla, A.; Singh, T. (2019). *Gene Expression Studies in AR/MTOR/MAPK Pathways in Prostate Cancer.* Journal of Integrative Bioinformatics, 16(3).
    [DOI] | [GitHub]
    R **GEO2R** **R/Shiny**