Avinash Karkada Ashok

Bioinformatics Engineer | Computational Biologist | Computational Structural Biology

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Summary

Computational biologist with 4+ years of experience spanning NGS pipeline development, transcriptomics and omics analysis, immune profiling, structural biology, molecular modeling, and reproducible computational research. Build and optimize analysis workflows using Python, R, Bash, Snakemake, Docker, Linux/HPC, and cloud platforms across academic and biotech settings. Experience includes influenza assay analytics, PhIP-Seq antibody profiling, RNA-seq and single-cell analysis exposure, epitope mapping, comparative genomics, molecular dynamics, and ML-supported data analysis.

Education

MS in Bioinformatics — Aug 2024 – May 2026
Johns Hopkins University — Baltimore, MD

BE in Biotechnology, First Class with Distinction — Jun 2019 – Jul 2023
Visvesvaraya Technological University — Karnataka, India

Experience

Bioinformatics Engineer — Sep 2024 – Present
Johns Hopkins University School of Medicine — Baltimore, MD

- Engineer and maintain computational pipelines for InFlux, a highly multiplexed NGS-based influenza A neutralization assay, including validation and QC workflows supporting strain-specific neutralization measurements across diverse patient cohorts in the Benjamin H. Larman Lab.
- Lead a PhIP-Seq antibody-profiling project analyzing serum samples to study microbial dysbiosis and humoral immunity in early-onset and late-onset colorectal cancer, polyp, and healthy control cohorts.
- Develop reproducible analysis workflows, statistical analyses, and publication-ready visualizations using Python, R, Bash, and HPC environments for large-scale serological and sequencing datasets.

Summer Bioinformatics Intern — Jun 2025 – Aug 2025
Infinity Bio, Inc. — Baltimore, MD

- Benchmarked and optimized NGS-based MIPSA analysis pipelines on AWS EC2 by evaluating alignment strategies and improving I/O handling, reducing runtime from approximately 24 hours to 6 hours and lowering compute time by approximately 75%.
- Contributed to EpitopeFindeR 2, a reproducible pipeline integrating FoldDisco-based structural mapping to identify continuous and discontinuous epitopes from library peptide sequences and localize antibody binding sites on 3D antigen structures.
- Built Latch Bio-based analysis workflows, including a UMAP-based sequence-space analyzer and visualization module, to improve usability for client-facing epitope mapping analyses.

Junior Research Fellow — Nov 2023 – Aug 2024
Indian Institute of Science — Bangalore, India

- Co-first-authored a comparative genomics study identifying mammalian adaptive signatures in clade 2.3.4.4b H5N1 across non-human hosts, highlighting convergent mutations relevant to human adaptation risk and genomic surveillance.
- Helped show that neuraminidase stalk length and haemagglutinin glycosylation patterns can bias segment pairing and promote reassortment routes linked to emergence of highly pathogenic clade 2.3.4.4b A(H5N1).
- Contributed to characterization of RHIM motifs in bat RNA viruses, including a SARS-CoV-2 Nsp13 RHIM, revealing species-specific ZBP1-RIPK3 cell death signaling.

Project Intern — Nov 2021 – Aug 2023
DRP Lab, Siddaganga Institute of Technology — Tumkur, India

- Performed molecular dynamics simulations of SAICAR synthase comparing Mg^{2+}-bound and apo states, revealing ion-dependent conformational changes; project received Best Undergraduate Thesis recognition.
- Assisted molecular dynamics and free-energy analyses of CETP mutants, showing structural distortions associated with reduced neutral lipid transfer efficiency.

Research Associate May 2020 – Aug 2023
Insilicomics Pvt. Ltd. Ooty, India

- Worked on molecular dynamics simulations, virtual screening, genome informatics, and statistical data analysis while building Python scripts, Bash workflows, and GUI tools for research use.
- Supported practical bioinformatics training programs and mentored students through hands-on computational biology workflows.

Summer Research Intern Aug 2022 – Nov 2022
NITTE University Mangalore, India

- Performed virtual screening of natural product libraries against LuxS, followed by docking, ADMET, and MD/MM-PBSA validation to nominate hits that could disrupt AI-2 signaling in Helicobacter pylori.
- Worked on computational and mixed experimental/computational studies involving MTAN inhibition, ferulic acid radioprotection, and piperine-AKT1 anticancer activity.

Summer Research Intern May 2021 – Oct 2021
Pristine Organics Bangalore, India

- Worked in R&D on dietary management approaches for patients with inborn errors of metabolic disorders.

Technical Skills

Programming and Platforms: Python, R, Bash, SQL, Java, Git, GitHub, Linux, Unix, HPC, SLURM, AWS, EC2, S3, GPU, Docker, Singularity, Conda, Mamba, Jupyter, R Markdown, Quarto, Shiny, VS Code, RStudio

Bioinformatics, Transcriptomics, and Omics: RNA-seq, scRNA-seq, transcriptomics, gene expression analysis, ChIP-seq, WGS, WES, PhIP-Seq, Biopython, Bioconductor, SAMtools, BCFtools, BEDTools, Bowtie, Bowtie2, BWA, Minimap2, Kallisto, Salmon, STAR, HISAT2, Cutadapt, Trimmomatic, FastQC, GATK, IGV, SRA Toolkit, BLAST, Clustal Omega, MAFFT, EMBOSS, CD-HIT, HMMER, edgeR, DESeq2, limma, Seurat, Scanpy, MEGA, IQ-TREE, comparative genomics, genome informatics, epitope mapping

Computational Biology and Data Science: pandas, NumPy, SciPy, scikit-learn, PyTorch, XGBoost, random-Forest, SVM, LASSO, PCA, UMAP, t-SNE, clustering, differential expression, enrichment analysis, pathway analysis, network analysis, statistical data analysis, sequence-space analysis

Workflow and Reproducibility: Snakemake, Latch, Docker, Singularity, Git, GitHub

Structural Biology, Docking, and Molecular Modeling: PyMOL, UCSF ChimeraX, Chimera, VMD, MODELLER, AlphaFold, ESMFold, Rosetta, HADDOCK, AutoDock, AutoDock Vina, GROMACS, AMBER, gmx_MMPBSA, FoldDisco, FoldX, Maestro, Schrödinger, CP2K, Gaussian, ORCA, RDKit, Open Babel, molecular dynamics, protein structure prediction, structural mapping, virtual screening, free-energy analysis, MM/PBSA, ADMET, protein-protein docking, protein-ligand docking, protein-DNA docking, nucleic acid docking, binder design

Visualization and Reporting: matplotlib, plotly, ggplot2, GraphPad Prism, Excel, PowerPoint, BioRender, LaTeX, R Markdown, Quarto, Shiny, Dash, Cytoscape, UCSC Genome Browser, Ensembl Genome Browser

Wet Lab Techniques: Cell culture, agarose gel electrophoresis, PCR, SDS-PAGE, Western blot, ICP-MS, sample handling and QC, ELISA

Selected Publications

Decoding non-human mammalian adaptive signatures of clade 2.3.4.4b H5N1 to assess its human adaptive potential
R. Nataraj, **A. K. Ashok**, A. A. Dey, and S. Kesavardhana
ASM Microbiology Spectrum

Bat RNA viruses employ viral RHIMs orchestrating species-specific cell death programs linked to Z-RNA sensing and ZBP1-RIPK3 signaling
S. Mishra, D. Jain, A. A. Dey, S. Nagaraja, M. Srivastava, O. Khatun, K. Balamurugan, M. Anand, **A. K. Ashok**, S. Tripathi, et al.
Cell iScience

Computational-driven discovery of AI-2 quorum sensing inhibitor targeting the 5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase (MTAN) to combat drug-resistant Helicobacter pylori
M. Kumar, **A. K. Ashok**, T. Bhat, K. Ballamoole, and P. Gollapalli
Computers in Biology and Medicine

High-throughput screening and molecular dynamics simulations of natural products targeting LuxS/AI-2 system as a novel antibacterial strategy for antibiotic resistance in Helicobacter pylori

A. K. Ashok, T. S. Gnanasekaran, H. S. S. Kumar, K. Srikanth, N. Prakash, and P. Gollapalli
Journal of Biomolecular Structure and Dynamics

Nrf2-regulated antioxidant response ameliorating ionizing radiation-induced damages explored through in vitro and molecular dynamics simulations
G. Tamizh Selvan, **A. K. Ashok**, A. S. J. Rao, P. Gollapalli, R. Vishakh, S. N. Kumari, and N. K. Chaudhury
Journal of Biomolecular Structure and Dynamics

Portfolio and Open-Source Highlights

- **InFlux Pipeline:** HPC-ready Snakemake/SLURM workflow for NGS-based influenza neutralization analysis covering barcode cleaning, anchored Cutadapt matching, QC, quantification, molecular-equivalence calculation, titration modeling, and 4PL outputs.
- **Influenza Antigenic Space:** Python/bash based H3N3 and H1N1 2D antigenic cartography mapping pipeline using MDS.
- **PhIP-seq Pipeline:** Developed and maintained a modular PhIP-seq antibody-profiling pipeline that integrates multi-library processing, MockIP-based background modeling/QC, statistical enrichment analysis, FDR hit calling, peptide annotation, and interpretable antigen-level reactivity outputs.
- **GROMACS-COLAB:** Jupyter notebooks for running molecular dynamics simulations in Colab environments.
- **MODELLER-GUI:** Tkinter-based GUI created to simplify MODELLER workflows for structure modeling.
- **PhIP-Seq-Pipeline-Installer:** Shell scripts developed to help new users install the PhIP-seq pipeline and key dependencies in the Larman Lab environment.
- Additional scripting and workflow utilities include GROMACS Bash helpers, XVG-to-RMS plotters, and average SDF calculators to simplify repetitive research tasks.

Certificates and Relevant Coursework

Certificates: Epigenetic Control of Gene Expression (University of Melbourne), SARS-CoV-2 Protein Modeling and Drug Docking (Coursera Project Network), Algorithms for DNA Sequencing (Johns Hopkins University), Drug Discovery (UC San Diego), Python for Genomic Data Science (Johns Hopkins University), Introduction to Genomic Technologies (Johns Hopkins University), Introduction to the Biology of Cancer (Johns Hopkins University), Summer School on Machine Learning in Bioinformatics (HSE University), Antibody Purification (Siddaganga Institute of Technology), Artificial Intelligence in Drug Discovery (CSIR-NEIST), Technical Hands-On Workshop: Molecular Docking (BDG Lifesciences)
Relevant Coursework: Introduction to Bioinformatics, Algorithms for Bioinformatics, Applied Machine Learning, Artificial Intelligence, Gene Expression Data Analysis and Visualization, Protein Bioinformatics, Practical Computer Concepts for Bioinformatics, Molecular Basis of Pharmacology, Molecular Biology, Epigenetics, Gene Organization and Expression, Genomic and Personalized Medicine, Biostatistics and Biomodelling, Biochemistry, Microbiology, Genetics and Genetic Engineering, Immunology and Immunotechnology, Biomolecular Simulations, Programming with Python, Genomics and Proteomics Data Analytics, Enzyme Technology, Clinical Trials and Data Management, Biopharmaceuticals and Regulatory Affairs

Awards and Service

Best Paper Presentation (JAIVIK 2022); Best Undergraduate Thesis; peer reviewer for Nature Communications, Journal of Crohn's and Colitis, Journal of Biomolecular Structure and Dynamics, and International Journal of Biological Macromolecules; mentored students in practical bioinformatics, molecular dynamics, and NGS analysis.