

PADAVINANGADY NAKUL BHAT

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Education

B. Tech (Hons.), Computer Science and Engineering (AI & ML)
Manipal Institute of Technology, Manipal, India

Jul. 2023—May 2027
CGPA: 8.56/10.00 (3.42/4.00)

Experience

Summer Research Fellow, Indian Institute of Science, Bengaluru May 2025—July 2025

- Selected for the prestigious IASc-INSA-NASI Summer Research Fellowship Program.
- Conducted research under Dr. Debnath Pal, Department of Computational and Data Sciences, focusing on the *GenetiGraph* project.
- Contributed to academic writing, software development, and project presentations related to genetic network analysis.

Undergraduate Researcher, Manipal Institute of Technology Jan 2024—Present

- Conducting interdisciplinary research across computational biology, machine learning, and data science, working on multiple ongoing projects and publications.
- Developing and maintaining the *GenetiGraph* library for modeling and visualizing genetic networks; currently collecting a dataset to validate the framework.
- Built the *ToxiTox* web platform for predicting chemical toxicity using fuzzy-matching pipelines.
- Authored a research paper on Chronic Kidney Disease (CKD) feature identification using statistical analysis and predictive modeling.
- Contributed extensively to research papers, technical presentations, and collaborative software development.

Mentors: Dr. S. Balaji (Biotech), Dr. Manoj T (CSE), Mr. Balaji B (MSIS), Dr. Krishnaraj C (CSE), Dr. Vinay M (Maths)

Skills & Tools

Programming Python, C, C++, Java, SQL, Shell Scripting	Machine Learning & XAI scikit-learn, Pytorch, XGBoost, SHAP, QLattice, imbalanced-learn	DevOps & Tools Git, GitHub Actions, CI/CD, Linux
Scientific Computing Computational Biology, Cheminformatics	Frameworks & Libraries pybind11, L ^A T _E X 2 _ε , Flask, RDKit	Core Skills Systems Design, Algorithms, Data Analysis

Projects

GenetiGraph: A Genetics Framework For AI Sep. 2024—Present

A framework for structured genetic inference and inheritance modeling in AI systems.

Tools: C++, Python, pybind11, L^AT_EX, Git, Github Actions

Skills: Systems design, CI/CD and Makefiles, library development, algorithm and data structure design

- Designed and implemented an efficient binodal mixed-graph data structure to represent complex genetic pedigrees, supporting remarriage, sibling ordering, and rich genotypic annotations. **[Patent Pending]**
- Invented a modular, partner-independent mathematical model enabling constant-time inheritance simulation across arbitrary family structures, with robust handling of incomplete or missing pedigree data. **[Preprint. Publication Pending]**

- Built and maintaining an open-source, cross-language genetic simulation library in C++ and Python, integrating the custom data structure and inheritance model, and exposing core algorithms via pybind11 for AI applications.
- Cut AI overhead in genetic inference by embedding probabilistic inheritance tracking in the simulation no more guessing missing links. Frees AI to focus on higher-level tasks like relation inference, phenotypic prediction, and linkage analysis with accurate multi-generational data.

ToxiTox: Structure-Based Toxicity Prediction [Restricted Disclosure]

Jul. 2024—Present

Building a new approach for predicting drug toxicity from molecular structures.

Tools: Python, Flask, RDKit, L^AT_EX, Git, PubChem API

Skills: Cheminformatics, Flask app development, SMILES encoding, fuzzy matching algorithms, cloud deployment

- Built and deployed a web app that predicts molecular toxicity classes and highlights toxic substructures using fuzzy matching.
- Integrated multiple input modes: single SMILES strings, structure drawing, and batch SMILES files for flexible molecule analysis.
- Used Flask and RDKit to generate molecular images and run structure-matching algorithms.
- Curating a custom toxicity dataset based on our structure-matching results to benchmark the tool.
- Writing papers to release the tool and dataset to the research community.

AI Framework for Hypothesis Generation in CKD Diagnosis [Under Review]

Aug. 2024—Present

AI-Powered Framework for Chronic Kidney Disease (CKD) Feature Identification and Hypothesis Generation

Tools: Python, scikit-learn, XGBoost, SHAP, ELI5, QLattice, pandas, NumPy, Matplotlib, Seaborn, Jupyter, Git, Linux

Skills: Machine Learning Model Evaluation, Explainable AI (XAI), Statistical Analysis, Clinical Data Analysis, Cross-Validation

- Evaluated 22 AI models in a multi-dataset study on CKD, selecting the best-performing model (99.5% accuracy) using Stratified K-Fold Cross-Validation.
- Applied explainable AI (XAI) methods (SHAP, ELI5, QLattice) and statistical methods to identify key features and data patterns.
- Designed the system to be model-agnostic and resilient across populations, and clinical contexts.
- Compared insights with clinical biomarkers to validate results and reveal potential novel indicators.

Publications

1. **Bhat, P. N.** and Pal, D. (2025). Genetic Expectations in Inheritance: A Probabilistic Algebraic Framework. *bioRxiv* Preprint. [\[Link\]](#). DOI:10.1101/2025.06.12.659255 Submitted to *Journal of Theoretical Biology*.
2. **Bhat, P. N.**, Balaji, S., and Shapshak, P. (2025). A Review of AI Tools in Molecular Biology and Virology. In *Global Virology V: 21st Century Vaccines and Viruses*. Springer Nature. Expected August 2025.

Under Review

1. **Bhat, P. N.**, Chadaga, K., and Sampathila, N. (2025). A Generalisable Explainable AI Framework for Biomedical Insight and Hypothesis Generation in Chronic Kidney Disease. Submitted to *Scientific Reports*.

Under Preparation

1. **Bhat, P. N.**[†], Badhri, B.[†], and Balaji, S. (2025). ToxiTox: A New Fuzzy-Matching Toxicity Predictor. *Under Preparation*. [†]Equal Contribution.
2. Lopez, A., **Bhat, P. N.**, Huang, D. L., Sahni, S., and Allamraju, A. (2025). Exploring the Relationship of Environmental, Social, and Governance (ESG) Scores on Firm Performance: An Empirical Analysis. *Under Preparation*.

Patents

1. **Bhat, P. N.** and Manoj, T. (2025). A System and Method for a Graph-Based Framework for Representing and Analysing Pedigree Charts. Published patent application. [\[Link\]](#)
2. **Bhat, P. N.** (2024). Iterative Imputation System and Method for Predicting Missing Environmental, Social, and Governance (ESG) Data. Published patent application. [\[Link\]](#)