

# Pritam Kumar Panda, Ph.D.

BIOINFORMATICS · DRUG DESIGNING · MOLECULAR MODELING · BIOPHYSICS · NEXT GENERATION SEQUENCING · MULTIOMICS

Department of Anesthesiology, Perioperative and Pain Medicine, Stanford, CA 94305

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📁 Portfolio 📄 Google Scholar 📄 Stanford Profile

## Professional Summary

Postdoctoral Scholar at **Stanford University** specializing in AI-driven protein design, molecular modeling, and drug development for advanced anesthetic solutions tailored to battlefield medicine. Skilled in bioinformatics workflows, high-throughput NGS data analysis, and workflow automation using Python, R, Bash, Nextflow, and Snakemake. Proven leader in managing large-scale datasets, optimizing computational pipelines, and mentoring interdisciplinary research teams. Adept at managing interdisciplinary teams, delivering scalable solutions, and translating research into real-world medical impact.

## Expertise

**Biophysics:** GROMACS, Umbrella Sampling, PCA & Gibbs Free energy, CHARMM-GUI, Steered MD simulations, Autodock4 & Vina, Nvidia DiffDock, AlphaFold2, ChimeraX, Schrödinger, DS Visualizer

**Genomics:** High throughput data analysis, WES/WGS/Variant calling (bwa-mem, GATK, Vardict, Mutect2, Deep Variant, IGV, VCF tools), Annotation (ANNOVAR, VEP, CADD), RNASeq (DESeq2, STAR), scRNASeq (Seurat, scanpy, cell ranger), Proteomics (FACS Analysis, CytoExploreR, IPA), Alignment & QC workflow, SNV Annotation, Nextflow/nf-core pipelines, Differential expression analyses, Single-cell omics & analysis across modalities, Spatial Transcriptomics, Flow Cytometry analysis, Ingenuity Pathway Analysis

**Data Science:** Machine Learning, AWS, HPC, Software Development

**Statistics:** Multimodal analysis, Multivariate analysis, Dimensionality reduction

**Quantum Physics:** VASP, Siesta, TranSiesta Electronic Transport, 2D Materials Modeling

**Soft Skills:** Project management, Documentatation/SOP, Public Speaking and Communication, Leadership, Multi-disciplinary Collaboration, Adaptive problem solving, Multi-tasking, Time Management, Technical Design, Self-Motivated, Strategic Planning, Critical Thinking, Teamwork

## Programming Skills

 Python

 R

 Bash

 Git

 CI/CD

 nf-core

 nextflow


 Singularity

 docker

 snakemake

 Flask

 Web Dev

 NodeJs

 AWS

 BioRender

## Work Experience

### Postdoctoral Scholar

STANFORD UNIVERSITY

California, USA

January 2025 - Present

- Spearheaded innovative research at the department of Anesthesiology, Perioperative and Pain Medicine, Stanford University School of Medicine focused on the design of battlefield-optimized anesthetics using AI-driven protein design, molecular dynamics simulations, and computational drug design to enhance anesthetic efficacy and adaptability in extreme conditions.
- Developed predictive frameworks through AI and molecular dynamics simulations, utilizing deep learning algorithms to assess protein structural variations and simulate anesthetic interactions at the atomic level, ensuring rapid response and resilience of anesthetics in field environments.
- Conducted molecular modeling of drug structures related to clinical anesthesia to analyze and predict biological activity, enhancing the precision of drug design for optimized anesthetic efficacy and targeted therapeutic outcomes.

- Implemented Quantitative Structure-Activity Relationship (QSAR) modeling to establish a quantitative link between molecular properties and pharmacodynamic attributes, improving safety and efficacy predictions and significantly reducing the need for initial testing in the development of novel anesthetic agents.

### **Bioinformatician**

GERMAN CANCER RESEARCH CENTER DKFZ

Heidelberg, Germany

July 2023 - Dec 2024

- Reduced NGS processing time by 40% by automating analysis pipelines (scRNAseq, RNAseq, WES, WGS) using Nextflow, Docker, and Singularity and ensured code integrity with GitLab/GitHub CI/CD pipelines.
- Perform exploratory data analysis and visualizations using R/Python to support needs for internal and collaborative data research projects.
- Managed large-scale big data projects, optimizing sequencing workflows with the DKFZ One Touch Pipeline database and leading multidisciplinary teams. Translating/piloting common bioinformatics tools to applications suitable for non-bioinformatics biologists and clinicians to query and interpret the molecular/clinical data.
- Implemented the HI-TRON data portal backend & frontend, enhancing data accessibility and user experience through MOLGENIS, VueJs and FAIR practices & and collect feedback and feature requirements from researchers including biologists, clinical trial designers and clinicians.
- Streamlined bioinformatics data processing by implementing parallelized workflows across high-performance computing (HPC) environments, resulting in a 30% increase in computational efficiency and faster data delivery for time-sensitive research projects.

### **Affiliated Researcher**

KAROLINSKA INSTITUTE

Stockholm, Sweden

March 2021 - March 2023

- Enhanced patient stratification and biomarker selection in clinical trials by developing novel predictive models using statistical techniques and machine learning on complex clinical data, including genomic data and antibody clones from patient samples.
- Advanced understanding of immunomodulatory effects in cardiovascular-related disorders by creating immunoinformatics pipelines for modeling in-house antibody clones, enabling antibody profiling and simulation.
- Improved visualization and accessibility of complex clinical data by designing exploratory data analysis pipelines using machine learning models for clinical data cohorts, enhancing data integration and usability.

### **Doctoral Researcher**

UPPSALA UNIVERSITY

Uppsala, Sweden

November 2018 - March 2023

- Developed a multi-scale modeling pipeline, enhancing computational efficiency and accuracy by utilizing molecular dynamics simulations on proteins, nanomaterials, complexes, and membrane models.
- Bridged quantum and biological behaviors of bio-inspired materials by establishing links to understand interface chemistry, focusing on 2D materials modeling.
- Led innovative sub-projects on ab-initio quantum methods, initiating, designing, and developing protocols using electronic transport models for DNA/protein nanopore sequencing and gas sensing mechanisms.

### **NGS Data Analyst**

UNIVERSITY MEDICAL CENTER, UNIVERSITY OF FREIBURG

Freiburg im Breisgau, Germany

September 2017 - October 2018

- Enhanced clinical diagnostics for Myelodysplastic Syndromes by developing and validating whole exome sequencing (WES) and NEBNext Direct clinical cancer hotspot panel pipelines, focusing on accurate variant identification and annotation.
- Optimized algorithm development in HPC environments, designing computing strategies that improved computational efficiency and accelerated research processes.
- Spearheaded a collaborative research project to design and analyze WES and gene-expression data using RNA-seq pipelines, leading to significant performance improvements.

## **Leadership and Outreach**

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### **Bioinformatics Consultant**

COLGATE AND PALMOLIVE

Piscataway-NJ, USA

November 2021 - June 2023 (Contract)

- Collaborated on developing a pipeline for combinatorial synergy-based drug design targeting photoaging and hyperpigmentation, which led to the publication of an article showcasing the innovative approach and findings. Demonstrated expertise in drug discovery research, with a strong focus on Computer-Aided Drug Design (CADD) methodologies and techniques.

## International Faculty Associate

KIIT SCHOOL OF BIOTECHNOLOGY

Bhubaneswar, India

August 2022 - January 2023 (Contract)

- Taught graduate-level courses in Bioinformatics and Systems Biology, conducting practical sessions to introduce students to current trends and concepts. Consistently received top reviews from both students and faculty for teaching excellence.

## Scientific Advisor

LONGHACK SPONSORED BY VITADAO

Helsinki, Finland

June 2021 - September 2022 (Contract)

- Guided and supported participants throughout the hackathon process, ensuring their understanding and addressing their needs effectively. Spearheaded the organization of two successful hackathons focused on longevity, showcasing strong leadership and project management skills. Played a key role in identifying potential customers and expanding networks, fostering valuable connections within the scientific and entrepreneurial communities through the hackathon platform.

## General Clinical Consultant

BREATH OF HEALTH

Cambridge, Massachusetts

November 2021 - December 2022 (Contract)

- Proficient in supporting the development of grant proposals, including clinical data analysis and bioinformatics data analysis, contributing to successful funding acquisition and research initiatives. Experienced in developing machine learning models and pipelines tailored for next-generation sequencing (NGS) data analysis and automation, optimizing workflows to enhance efficiency and accuracy in genomic research.

## Founder and CEO

NERDALYTICS

Uppsala, Sweden

December 2021 - July 2023

- Founded a project management startup specializing in bioinformatics consultancy for pharmaceutical industries, aligning services with industry demands. Adapted company policies, regulations, and financial strategies to effectively manage multiple projects, ensuring long-term viability and sustainability. Led budgeting, coordination, and development of confidential projects with pharmaceutical companies, focusing on defining project scope, cost estimation, and key deliverables.

## Scientific Advisor and Bioinformatician

INFLANOVA AB

Stockholm, Sweden

August 2021 - March 2023 (Contract)

- Played a pivotal role in identifying potential clients within industrial sectors interested in vaccine formulation by leveraging market research and networking skills to establish connections and initiate discussions with prospective partners. Filed a patent **WO2023217787** for a clinical vaccine candidate targeting antiviral therapy. Utilized multiomics and bioinformatics approaches to develop innovative strategies for vaccine design and therapeutic interventions.

## Core Competencies

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- Applied data science techniques within high-performance computing (HPC) and AWS cloud environments to optimize computational workflows for molecular dynamics, protein modeling, and drug design projects.
- Proficient in molecular dynamics simulations and advanced sampling techniques such as Umbrella Sampling and Principal Component Analysis (PCA) for calculating Gibbs free energy, utilizing CHARMM-GUI for precise molecular modeling and steered MD simulations.
- Experienced in molecular docking and protein structure prediction through tools like Autodock4, Vina, Nvidia DiffDock, and AlphaFold2, complemented by expertise in visualizing molecular interactions using ChimeraX, Schrödinger, and DS Visualizer for enhanced research insights.
- Conducted high-throughput genomic data analysis across multiple modalities, including SNV Annotation, Differential Expression Analyses, and Single-cell Omics, using robust pipelines (Nextflow/nf-core) for streamlined workflow and reproducibility.
- Skilled in advanced statistical techniques for handling large and complex biological datasets, leveraging multimodal, multivariate, and dimensionality reduction methods to derive meaningful insights from high-dimensional data.
- Performed Spatial Transcriptomics and Flow Cytometry analysis to uncover complex biological pathways, utilizing Systems Biology approaches with Ingenuity Pathway Analysis for comprehensive understanding of cellular interactions and therapeutic targets.
- Excelled in communicating complex scientific findings and computational strategies to non-technical stakeholders, ensuring project alignment and securing support from cross-departmental teams and external collaborators. Adapted and implemented agile project management practices to improve project efficiency and accountability.

## Publications

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Please refer to my **Google Scholar** for a full publications list.

- Panda, P. K. ; Arul, M. N. ; Patel, P. ; Verma, S. K. ; Luo, W. ; Rubahn, H.-G. ; Mishra, Y. K. ; Suar, M. ; Ahuja, R. Structure-Based Drug Designing and Immunoinformatics Approach for SARS-Cov-2. **Science advances (AAAS)** 2020, 6 (28), eabb8097
- Panda, P. K., Kumari, P., Patel, P., Samal, S. K., Mishra, S., Tambuwala, M. M., ... & Verma, S. K. (2022). Molecular nanoinformatics approach assessing the biocompatibility of biogenic silver nanoparticles with channelized intrinsic steatosis and apoptosis. **Green Chemistry**, 24(3), 1190-1210.
- Sahoo, S. S. ; Pastor, V. B. ; Goodings, C. ; Voss, R. K. ; Kozyra, E. J. ; Szvetnik, A. ; Noellke, P. ; Dworzak, M. ; Stary, J. ; Locatelli, F. ; Panda, P. K. ; others. Clinical Evolution, Genetic Landscape and Trajectories of Clonal Hematopoiesis in Samd9/samd9l Syndromes (Vol 27, Pg 1806, 2021). **Nature Medicine** 2021, 27 (12), 2248–2249
- Krombholz, C. F. ; Gallego-Villar, L. ; Sahoo, S. S. ; Panda, P. K. ; Wlodarski, M. W. ; Aumann, K. ; Hartmann, M. ; Lipka, D. B. ; Daskalakis, M. ; Plass, C. ; others. Azacitidine Is Effective for Targeting Leukemia-Initiating Cells in Juvenile Myelomonocytic Leukemia. **Nature Leukemia** 2019, 33 (7), 1805–1810
- Loyola, V. P. ; Panda, P. K. ; Sahoo, S. S. ; Szvetnik, E. A. ; Kozyra, E. J. ; Voss, R. K. ; Lebrecht, D. ; Wehrle, J. ; Erlacher, M. ; Stary, J. ; others. Monosomy 7 as the Initial Hit Followed by Sequential Acquisition of Setbp1 and Asx11 Driver Mutations in Childhood Myelodysplastic Syndromes. **Blood** 2018, 132, 105–106
- Simnani, F. Z. ; Singh, D. ; Patel, P. ; Choudhury, A. ; Sinha, A. ; Nandi, A. ; Samal, S. K. ; Verma, S. K. ; Panda, P. K. Nanocarrier Vaccine Therapeutics for Global Infectious and Chronic Diseases. **Materials Today** 2023, 66. 371-408
- Bhardwaj, V., Handler, M. Z., Mao, J., Azadegan, C., Panda, P. K., Breunig, H. G., ... & König, K. (2024). A novel professional-use synergistic peel technology to reduce visible hyperpigmentation on face: Clinical evidence and mechanistic understanding by computational biology and optical biopsy. **Experimental dermatology**, 33(4), e15069.
- Sahoo, B. R., Panda, P. K., Liang, W., Tang, W. J., Ahuja, R., & Ramamoorthy, A. (2021). Degradation of Alzheimer's amyloid- $\beta$  by a catalytically inactive insulin-degrading enzyme. **Journal of molecular biology**, 433(13), 166993.

## Conferences

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- Participated in 1st Helmholtz Health Summit “The Future of Medicine”, Berlin, Germany, 2024
- Data Symphony: Orchestrating Pseudonymization and Seamless Transfers Across HI-TRON Mainz, HITRON Symposium, Mainz, Germany, 2024
- Participated in Curious2024 - Future Insight conference, Mainz, Germany, 2024
- SAMD9 and SAMD9L Germline Disorders in Patients Enrolled in Studies of the European Working Group of MDS in Childhood (EWOG-MDS): Prevalence, Outcome, Phenotype and Functional Characterisation, Blood, Volume 132, Supplement 1, 2018, Page 643
- Monosomy 7 As the Initial Hit Followed By Sequential Acquisition of SETBP1 and ASXL1 Driver Mutations in Childhood Myelodysplastic Syndromes, Blood, Volume 132, Supplement 1, 2018, Page 105
- Participated in European Working Group of Myelodysplastic Syndrome (MDS) and Severe Aplastic Anemia (SAA) in children and adolescents (2018)

## Key Achievements/Recognitions

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- Nominated and accepted as a member of **Sigma Xi, The Scientific Research Honor Society**.
- Appointed as **Nextflow Ambassador** by Nextflow (Seqera) and nf-core community.
- Over **10K+** engaged followers on **LinkedIn**, sharing insights on bioinformatics, molecular modeling, drug designing, NGS analytics, and scientific workflows.
- Reviewed more than 30 proposals for Biotechnology Industry Research Assistance Council (BIRAC).
- Received a research grant from **Colgate & Palmolive** to conduct computer-aided drug design (CADD) studies.
- Acknowledged by Elsevier and Springer for outstanding contributions as a reviewer.
- Two times Chairperson at the **e-Materials Research Society** conference.
- Received **IMM Strategic Interdisciplinary** Collaboration Grant at Karolinks Institute.
- Awarded AIMday materials 2020 grant (Uppsala University innovation grant) by ABB Power Grids, Hitachi, Sweden.
- Invited as a guest for exclusive one-on-one conversations by leading **TV news** channels in India.
- Featured in The **The Global Indian** for featuring my journey in its exclusive series ‘Indians in Europe’.

## Teaching and Mentorships

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- Mentored, managed, and drove a team of 160 researchers from 10 different countries to organize a longevity hackathon.

- Initiated a startup with strong initiative, ownership, and accountability for innovative projects.
- Providing hands-on training on YouTube related to NGS, computer-aided drug designing, quantum chemistry methods, molecular dynamics, and bioinformatics lectures.
- Instructed Master's level courses at KIIT University, India, crafted comprehensive lesson plans, delivered engaging lectures, and conducted interactive discussions to enrich student comprehension of the curriculum.

## Certifications

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- Stanford Online:** Machine Learning Specialization
- Coursera:** Google Data Analytics
- Amazon:** AWS Technical Essentials
- QIAGEN:** QIAGEN Ingenuity Pathway Analysis
- Udemy:** Designing nano devices and sensors, 100 Days of Code: The Complete Python Pro Bootcamp
- Six Sigma:** Six Sigma Green Belt by International Six Sigma Institute
- EMBL-EBI/GHGA:** Nextflow, nf-core hackathon, RNAseq, scRNASeq
- DKFZ:** Cyber Security, Good Scientific Practices, Prevention of Corruption, Medical Laboratories Quality and Competence

## Education

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### Ph.D. in Physics (Specialization in Atomic, Molecular and Condensed Matter Physics)

UPPSALA UNIVERSITY

Uppsala, Sweden

November 2018 - March 2023

### Master of Technology in Bioinformatics

D Y PATIL UNIVERSITY

Mumbai, India

July 2014 - August 2016

### Master of Science in Bioinformatics

UTKAL UNIVERSITY

Bhubaneswar, India

July 2012 - August 2014

### Bachelor of Science in Bioinformatics

UTKAL UNIVERSITY

Bhubaneswar, India

July 2009 - August 2012