ROHIT NANDAKUMAR

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EDUCATION

Carnegie Mellon University
Master of Computational Biology (GPA: 3.72/4.0)   **May 2025**

Arizona State University
Bachelor of Biomedical Informatics (GPA: 4.0/4.0)   **May 2022**

EXPERIENCE

Isayev Lab at Carnegie Mellon University   **09/2023 – Present**
Computational Drug Discovery Researcher   *Pittsburgh, PA*
- Developed an ultra-scalable SMILES-based GNN, enabling billion-scale chemical property prediction for drug discovery, battery electrolytes, green chemistry, and aerospace materials.
- Achieved 50x scalability over SOTA models, training 20M molecules in just 15 min/epoch on a single GPU and 10GB CPU RAM—reducing R&D compute costs and experimental bottlenecks.

Computational Biology Intern at Predictive Oncology   **05/2024 – 08/2024**
Computational Biology Intern   *Pittsburgh, PA*
- Built an ML pipeline for high-dimensional Cell Painting data, accelerating biomarker discovery for precision medicine.
- Enabled patient-specific drug response predictions, revealing individual variations within the same cancer subtype, driving personalized oncology advancements.

Dinu Lab at Mayo Clinic   **01/2020 – Present**
Student Research Assistant   *Scottsdale, AZ*
- Developed an AI-driven multi-omics framework for diagnosing developmental dyslexia, integrating clinical, genomic, and metabolic data, achieving 86% accuracy (AUC = 0.83)

Independent Computational Drug Discovery Researcher   **08/2017 – 12/2020**
Independent   Chandler, AZ
- Developed a high-precision ML model to identify protein hotspots, discovering small molecules targeting the EphB2-EphrinB2 complex (gastrointestinal cancers).
- Published first-author research, achieving AUROC 0.842, ranking among top-performing PPI-based models.
- Identified nadolol as a potential drug repurposing candidate for gastrointestinal cancer.

Keats Lab at Translational Genomics Research Institute (TGen)   **06/2019 – 08/2019**
Helios Scholar Intern   Phoenix, AZ
- Crafted an algorithm that could differentiate optical and PCR duplicates on Illumina Next-Generation Sequencing (NGS) sequencing machines 4.5x faster compared to state-of-the-art by the Broad Institute at Harvard and MIT

PUBLICATIONS

Rohit Nandakumar, *Valentin Dinu*. *Developing a machine learning model to identify protein–protein interaction hotspots to facilitate drug discovery.* *PeerJ, December 2020*.

SKILLS

Languages/Tools: *Pytorch, Python, R, scikit-learn, Pandas, Keras, git, NumPy, samtools, Picard/GATK, rdkit, PyMol*
Technologies/Frameworks: *High Performance Computing (HPC), Next Generation Sequencing (NGS)*