Shantanu Khatri, Sr. Research Fellow
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Professional Summary

Computational Biologist with extensive experience in protein structural modeling, molecular dynamics simulations, and **AI/ML** leveraging **high-performance computing**. Proficient in **high-throughput data analysis** and adept at designing and developing **holistic *in silico* workflows**.

Education

- **Ph.D., Computational Biology**
  Council of Scientific and Industrial Research–Institute of Genomics and Integrative Biology, New Delhi, India (2020–Present)
  Thesis: Understanding Conjugation Machinery in Human Autophagic System
  Advisor: Dr. Lipi Thukral
- **Master of Science** (M.Sc.), Biological Science (2013 - 2015)
  Hemvati Nandan Bahuguna Garhwal University, Uttarakhand, India
- **Bachelor of Science** (B.Sc.) Biological Science (2010 - 2013)
  Hemvati Nandan Bahuguna Garhwal University, Uttarakhand, India

Technical Expertise

- Multiscale protein modeling and analysis of protein dynamics and interactions in high-order assemblies and protein–membrane systems using molecular dynamics simulations, including coarse-grained and all-atom approaches with GROMACS, CHARMM, and OpenMM.
- Protein modeling with AI based pipelines **AlphaFold, RFdiffusion, CHAI, BoLTZ** and performing protein-ligand docking with **HADDOCK and AutoDock**.
- Visualizing and presenting molecular structures using **ChimeraX, PyMOL, VMD, and Blender.**
- Free Energy Calculations (MM-PBSA, Poisson–Boltzmann Surface Area) and analyzing protein structural networks in high-order oligomers.
- Scripting and automating computational workflows with **Python, Unix, and Bash**, utilizing libraries like **Pandas, Scikit-learn, NumPy, Biopython and MDAnalysis.**
- High throughput data analysis on large-scale computations with high-performance computing tools like **SLURM, LSF and PBS, CSIR-IGIB (Tejas), CSIR-4PI (Ananta), CDAC (BRAF), IBDC, and AWS cloud.**
- Containerization using **Docker and Singularity on CPU/GPU (NVIDIA DGX** Platform), executing scientific and drug discovery workflows on AWS.
- Experimental design and validation techniques, **including ITC and protein purification**, to support and corroborate computational findings.
- Building and optimizing pipelines for **multi-omics** data integration and analysis using python/R based scientific libraries.
- Database management and web resource development for bioinformatics resources.
- **Proficient in developing AI/ML and deep learning** workflows for bioinformatics and biological data analysis**.**
- Experience in version control systems, including **Git and GitHub**. **VS Code IDE** for scripting and collaborative development.

Research Projects

- Leveraged **AlphaFold2-Multimer** to predict high-order oligomeric assemblies regulating conjugation machinery in human autophagy and performed microsecond molecular simulations to analyse protein structural dynamics.
- Investigated structural differences in various functional forms of **E1 enzyme ATG7** by leveraging AlphaFold to generate assemblies and performing molecular dynamics simulations to map critical interactions with key proteins such as LC3B, ATG12, ATG3 and ATG10. Validated these interactions through **in-silico mutagenesis and invitro biophysical experiments** (ITC).
- Explored the bipartite **membrane protein ATG2A**, revealing its architecture, and identified dynamic transitions of cavity-lining residues through simulations, suggesting their critical role in regulating lipid transfer (Developed an in-house analysis script to characterize these transitions and extract cavity-residue dynamics).
- Developed **web-resource** RAPSAP (Resource of AlphaFold2 Predicted Structures of Autophagy Pathway), a curated database providing comprehensive structural information on the complete human autophagy protein interactome.

Publications

- Malhotra Nidhi[#], **Shantanu Khatri[#]**, Ajit Kumar, Akanksha Arun, Purba Daripa, Saman Fatihi, Sureshkumar Venkadesan, Niyati Jain, and Lipi Thukral. "AI-based AlphaFold2 significantly expands the structural space of the autophagy pathway." ***Autophagy*** **19, no. 12 (2023): 3201-3220**. **[#]equal contribution.**
- **Shantanu Khatri**, Shruti Mathur, Lipi Thukral, Deciphering ATG7's multifaceted structural landscape in human autophagic conjugation system, 2025. (In preparation)
- Mapping the functional terrain of E1-like ATG7: Insights into cross-functional roles, **Shantanu Khatri**, Lipi Thukral 2025. (Review, In preparation)

Awards & Recognitions

- Council of Scientific & Industrial Research-National Eligibility Test: Junior Research Fellowship (June 2019)
- Council of Scientific & Industrial Research-National Eligibility Test: Lectureship (December 2018)
- Selected as Springer Nature Student Ambassador (2023)
- Recognition By Springer Nature for contribution in the 'Her Research, Our Future' Forum: 21 March 2024

Invited Talks, Conferences & Workshops

- Invitation: Delivered a research seminar at the invitation of Prof. Alexandre Bonvin (Professor of Computational Structural Biology), **HADDOCK, Utrecht University, The Netherlands** (May 2025)
- Poster: '*AI-based AlphaFold2 significantly expands the structural space of the autophagy pathway*' EMBO Workshop on **Computational Structural Biology, EMBL, Heidelberg, Germany** (Dec 2023)
- Poster: '*Autophagy pathway'* 63rd Research Council Meeting, CSIR-IGIB, (Nov 2023)
- Delegate: Mini symposium on 'Latest in Autophagy and Lysosome Biology' at CSIR-IGIB: 12 January 2023

- Delegate: Symposium on 'Data Driven Approaches to Understand Biological Systems at Bioinformatics Centre', CSIR-IGIB, New Delhi: 29 April 2023

Courses/ Certificates

- **Fundamentals of AI/ML in Precision Medicine:** Course by the **Department of Genetics, Stanford Medicine**, covering topics such as machine learning algorithms, multiomics data integration, predictive modeling, and AI applications in healthcare.

- **Fundamentals of Data Science in Precision Medicine and Cloud Computing:** Course by the **Department of Genetics, Stanford Medicine, focused on multi-omics data analysis, cloud-based workflows**, computational pipelines, and data-driven insights in precision medicine.

- **Deep learning with Pytorch ,** python-first framework.

Volunteer Work & Leadership

- Organizer: **AWS Workshop-Biology on Cloud** at CSIR-IGIB, New Delhi, 6 November 2023.
- Co-Organizer: Science Entrepreneurship Competition (IGIB BIG Ideas), November 2023
- Project Coordinator: 'Bringing Genomics Closer to Society' an audiovisual project as a part of One Week, One Lab at CSIR-IGIB.
- Organizer: Interactive Discussion on 'Women in STEM' as part of Springer Nature IWD 2024
- Volunteered in International Workshop," Applications of AI and Data-Driven Approaches in Structural Biology 2024, CSIR-IGIB.

Extra-Curricular Activities

- Active participation in institutional-level tournaments for table tennis, cricket, and badminton, with awards including Runner-up in National CSIR-SSBMT Table Tennis Tournament
- Fitness Drive 2022 Runner-up & Fitness Drive 2024 Winner in Table Tennis Tournament, CSIR-IGIB.

Languages

- English (Fluent/Professional Proficiency)
- Hindi (Native Proficiency)
