

Shri Kant, PhD

Computational Biology

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OBJECTIVE:

To advance our understanding of biomolecular recognition through the integration of structural biology, molecular simulations, machine learning, and bioinformatics, and to develop computational methods and resources that enable discoveries in RNA biology, protein–nucleic acid interactions, and data-driven life sciences.

RESEARCH OVERVIEW

Computational structural biologist with expertise in protein–RNA interactions, molecular recognition, molecular dynamics simulations, structural bioinformatics, machine learning, and high-performance scientific computing. Experienced in developing computational methods, structural datasets, and bioinformatics resources to investigate biomolecular interactions and conformational dynamics. Strong background in Python-based scientific programming, large-scale data analysis, and interdisciplinary research at the interface of structural biology, data science, and artificial intelligence.

Research Expertise

- Protein–RNA recognition, conformational selection, and induced-fit mechanisms.
- Development of non-redundant structural benchmarks and datasets for biomolecular interactions.
- Construction and analysis of backbone-dependent and secondary-structure-dependent rotamer libraries.
- Machine learning and statistical approaches for predicting nucleic-acid binding sites and biomolecular interactions.
- Multi-microsecond molecular dynamics simulations and conformational ensemble analysis of protein–RNA systems.
- Structural and functional characterization of DNA-, RNA-, and dual-binding proteins.
- High-performance computing (HPC), scientific workflow development, and large-scale biomolecular data analysis.

ACADEMICS

Degree	Institute / Details	Thesis / Dissertation
Ph.D.		
Computational Biology		
2018–2026	Indian Institute of Technology Kharagpur, India	<i>Conformational analysis of protein–RNA recognition</i>
M.Tech.		
Computational Biology		
2014–2016		
CGPA: 8.2/10	Anna University, Chennai	<i>In silico approach towards understanding the mechanism of action of metformin in type II diabetes mellitus</i>
B.Pharm.		
2010–2014		
74%	Guru Ghasidas Central University, Bilaspur, Chhattisgarh	<i>Library dissertation on brain learning power</i>
HSC		
2008–2010		
84.2%	CGBSE, Raipur, Chhattisgarh	–
HS		
2006–2008		
60%	CGBSE, Raipur, Chhattisgarh	–

PUBLICATIONS

1. **Kant S**, Chandran N, Mukherjee S, Maity A, Bahadur RP. (2025). *Protein-RNA Docking Benchmark v3.0 integrated with Binding Affinity. Proteins: Structure, Function and Bioinformatics*. DOI: [10.1002/prot.26825](https://doi.org/10.1002/prot.26825)
2. Agarwal A, **Kant S**, Bahadur RP. (2023). *Efficient mapping of RNA-binding residues using local sequence features in protein-RNA complexes. Proteins: Structure, Function and Bioinformatics*. DOI: [10.1002/prot.26528](https://doi.org/10.1002/prot.26528)
3. Verma J, Jain D, Panda AP, **Kant S**, Kumar G, Ghosh AS. (2023). *Involvement of non-active site residues in the catalytic activity of NDM-4 Metallo beta-lactamase. Protein Journal*. DOI: [10.1007/s10930-023-10124-6](https://doi.org/10.1007/s10930-023-10124-6)
4. Agarwal A, Alagar S, **Kant S**, Bahadur RP. (2023). *Binding dynamics of tandem RNA recognition motifs (tRRMs) of HuR with mRNA. J. Biomol. Struct. Dyn.* DOI: [10.1080/07391102.2022.2073270](https://doi.org/10.1080/07391102.2022.2073270)
5. Agarwal A, Singh K, **Kant S**, Bahadur RP. (2022). *Comparative analysis of machine learning classifiers for predicting protein-binding nucleotides in RNA sequences. Comput. Struct. Biotechnol. J.* DOI: [10.1016/j.csbj.2022.06.036](https://doi.org/10.1016/j.csbj.2022.06.036)

PUBLICATIONS UNDER REVISION OR COMMUNICATION

1. Mukherjee S, **Kant S**, Bahadur RP. (2025). *Transition of side-chain conformations of RNA-binding proteins upon binding RNA. [Submitted at Nucleic Acids Research].**
2. **Kant S**, Masipeddi S, Bahadur RP. (2025). *Deciphering conformational preferences of RNA in protein-RNA recognition. [Under revision by RNA Journal].*
BioRxiv: <https://doi.org/10.64898/2026.05.14.725147>.
3. **Kant S**. *Decoding Mutually Induced Conformational Changes in Non-Canonical Recognition of U1 SL4 snRNA by ULD of SF3A1 during Early Spliceosome Assembly. [Under revision by Journal of Molecular Recognition]*
BioRxiv: <https://doi.org/10.64898/2026.03.30.715355>.
4. Bhagat M, **Kant S**, Bahadur RP. (2026). *Structural dissection of the DNA- and RNA-binding protein (DRBP) complexes. [Under preparation].**
5. Garai S, **Kant S**, Bahadur RP. (2026). *TF-NRD: Transcription Factors non-Redundant Sequence and Structure Dataset. [Under revision by Journal of Structural Biology].*

* Equally contributed and joint first authors.

RESEARCH PROJECTS

PhD, Indian Institute of Technology Kharagpur, India

Dept. of Bioscience & Biotechnology – Advisor: Prof. Ranjit P. Bahadur

Title: *Conformational analysis of protein-RNA recognition*

Key Contributions:

- Developed a non-redundant protein-RNA docking benchmark with integrated binding affinity.
- Designed secondary structure-dependent and backbone-dependent rotamer libraries specific to RNA-binding proteins.
- Curated a library of RNA conformers for enhanced structural modelling and prediction.
- Investigated conformational changes in RNA-binding proteins upon RNA interaction.

Structural Characterisation of DNA- and RNA-Binding Proteins (DRBPs)

- Analysed DRBP structural interfaces using non-redundant datasets from RCSB PDB.
- Compared dual-binding interfaces of DRBPs with RBPs and DBPs.

Master of Technology, Anna University Chennai, India

Centre for Biotechnology – Advisor: Prof. B.S. Lakshmi

Title: *In silico approach towards understanding the mechanism of action of metformin in type II diabetes mellitus.*

COMPUTATIONAL SKILLS

- **Bioinformatics skills:** BLAST, CLUSTAL, NACCESS, US-align, TMalign, MMseqs2, HBPLUS, DSSP, MODELLER
- **Programming:** Python, Shell scripting, R, C
- **Machine Learning:** Scikit-learn, PyTorch
- **Molecular Dynamics:** AMBER, GROMACS
- **Visualisation :** PyMOL, ChimeraX, VMD, Coot
- **Operating Systems:** Linux (Ubuntu, CentOS), Windows, macOS
- **Web Development:** Django web-server, HTML, PHP, CSS, MySQL, Apache

HIGH-PERFORMANCE SCIENTIFIC COMPUTING (HPSC) EXPERIENCE

- Proficient in Slurm-based job scheduling and parallel computing on HPC clusters.
- Extensive experience using IIT Kharagpur's [Paramshakti Supercomputer](#) for large-scale molecular dynamics simulations.
- Participated in multiple National Super Computing Mission (NSM) workshops on HPC optimisation and system utilisation.

AWARDS AND ACHIEVEMENTS

- Travel Grant – RNA India meeting (2026), IISc, Bengaluru
- Travel Grant – EMBL Heidelberg Conference on the Expanding World of RBPs (2025)
- Fully Funded Participant – EMBO Workshop on Computational Structural Biology (2023)
- Institute Research Fellowship – IIT Kharagpur
- AIR-4 – DBT Computational Biology Entrance Exam (Pondicherry Centre)
- Registered Pharmacist – Chhattisgarh Pharmacy Council

CONFERENCES: POSTER PRESENTATION

- **13th RNA India meeting** – IISc, Bengaluru (Apr 27–29, 2026)
 - Poster: *Deciphering conformational preferences of RNA in protein-RNA recognition*
 - Poster: *Decoding mutually induced conformational changes in non-canonical recognition of U1 SL4 snRNA by the SF3A1 ULD during early spliceosome assembly*
- **EMBL Conference: The Expanding World of RBPs** – Heidelberg, Germany (Mar 11–14, 2025)
 - Poster: *RNA Conformational Preferences in Protein-RNA Recognition*
 - Poster: *Structural analysis of proteins involved in binding both DNA and RNA*
- **Horizons in Structural and Computational Biology 2025** – IIT Hyderabad (Feb–Mar 2025)
 - Poster: *Unveiling DNA- and RNA-binding proteins: Structural Insights and Interaction Dynamics*
- **EMBO Workshop on Computational Structural Biology** – EMBL Heidelberg, Germany (Dec 6–9, 2023)
 - Poster: *The Role of RNA Conformational Transition in Protein-RNA Recognition*

MENTORSHIP AND TEACHING

- **Mentor:** Master's Thesis, Computational Structural Biology, IIT Kharagpur
- **Teaching Assistant:** Computational Structural Biology & Bioinformatics Lab

SOFT SKILLS

- Strong analytical and problem-solving abilities
- Effective written and verbal communication
- Team collaboration and interdisciplinary coordination
- Adaptability to new computational environments
- Critical thinking and attention to detail
- Project planning and time management
- Mentoring and guiding junior researchers
- Perseverance and commitment to continuous learning

References

- 1. Prof. Ranjit P. Bahadur (PhD Supervisor)**
Professor, Computational Structural Biology Lab
Department of Biotechnology
Indian Institute of Technology Kharagpur, India
Email: r.bahadur@bt.iitkgp.ac.in
- 2. Dr. Nithin Chandran**
Assistant Professor (Adjunct), Laboratory of Computational Biology
Biological and Chemical Research Centre
University of Warsaw, Poland
Email: n.chandran@uw.edu.pl
- 3. Dr. Sunandan Mukherjee**
Department of Public Health, Section for Health Data Science and AI
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DECLARATION

The information provided above is true to the best of my knowledge.

Shri Kant

Date: August 25, 2026

Place: Bangalore, India