

Curriculum Vitae

Dr. Sunandan Mukherjee

1 Personal Information

Date of Birth: May 16, 1986
Nationality: Indian
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2 Academic Qualifications

Ph.D., Computational Structural Biology 2012–2018

Indian Institute of Technology Kharagpur, India

Thesis: Understanding Structural and Physicochemical Basis of Protein-RNA and Protein-Protein Interactions

Focused on molecular dynamics simulations and structural modeling for protein-RNA/protein interactions.

M.Sc., Bioinformatics 2007–2009

Lovely Professional University, Punjab, India

Thesis: Insilico drug designing for breast cancer for BRCA-1 mutated carrier

B.Sc., Microbiology (Honours) 2004–2007

Bankura Sammilani College, University of Burdwan, India

3 Professional Experience

Postdoctoral Researcher 07/2018–Present

Laboratory of Bioinformatics and Protein Engineering, IIMCB, Warsaw, Poland

- Developed SimRNA-Cry for RNA 3D structure prediction using cryo-EM data.

- Collaborated with experimental groups to validate computational models.

Internal In-Depth Tester 12/2023–Present

Nucleic Acids Research, Oxford University Press

- Evaluated web server issues for nucleic acid research platforms.

Protein Engineering Specialist 05/2022–10/2022

InCircular BV, Amsterdam, Netherlands & IIMCB, Poland

- Conducted Monte Carlo dynamics simulations to assess protein thermal unfolding.

Institute Teaching Assistant 01/2016–01/2018

Department of Biotechnology, IIT Kharagpur, India

- Taught bioinformatics and computational structural biology courses.

Junior Research Fellow 06/2011–10/2011

All India Institute of Medical Sciences, New Delhi, India

- Evaluated real-time PCR assay for Chlamydia trachomatis detection.

4 Selected Publications (Full list available on Google Scholar and ORCID)

1. Biela AD, ..., Mukherjee S, *et al.* (2025). "Determining the effects of pseudouridine incorporation on human tRNAs." *EMBO Journal* (In press).
2. Kant S, Nithin C, Mukherjee S, *et al.* (2025). "Protein-RNA docking benchmark v3.0 integrated with binding affinity." *Proteins: Structure, Function, and Bioinformatics* (In press).
3. Bu F, ..., Mukherjee S, *et al.* (2025). "RNA-Puzzles Round V: Blind predictions of 23 RNA structures." *Nature Methods*, 22, 399–411. doi.org/10.1038/s41592-024-02543-9.

4. Mukherjee S, *et al.* (2024). “Advances in the field of RNA 3D structure prediction and modeling, with purely theoretical approaches, and with the use of experimental data.” *Structure*, 32(11), 1860–1876. doi.org/10.1016/j.str.2024.08.015.
5. Rocha de Moura T, ..., Mukherjee S, *et al.* (2024). “Conserved structures and dynamics in 5′-proximal regions of Betacoronavirus RNA genomes.” *Nucleic Acids Research*, gkae144.
6. Niemyska W, Mukherjee S, *et al.* (2024). “Discovery of a Trefoil Knot in the RydC RNA: Challenging Previous Notions of RNA Topology.” *Journal of Molecular Biology*, 436(6).
7. Cappannini A, ..., Mukherjee S, *et al.* (2024). “MODOMICS: a database of RNA modifications and related information. 2023 update.” *Nucleic Acids Research*, 52(D1), D239–D244.
8. Chojnowski G, ..., Mukherjee S, *et al.* (2023). “RNA 3D structure modeling by fragment assembly with small-angle X-ray scattering restraints.” *Bioinformatics*, 39(9), btad527.
9. Luo B, ..., Mukherjee S, *et al.* (2023). “Cryo-EM reveals dynamics of Tetrahymena group I intron self-splicing.” *Nature Catalysis*, 6, 298–309.
10. Jia X, ..., Mukherjee S, *et al.* (2023). “Structural basis of sRNA RsmZ regulation of *Pseudomonas aeruginosa* virulence.” *Cell Research*, 33, 328–330.

5 Skills and Expertise

Computational & Molecular Modeling:

- Advanced 3D structural modeling of nucleic acids and protein complexes.
- Molecular dynamics (Amber), Monte Carlo, and free energy calculations.
- Developed SimRNA-Cry for RNA structure modeling with cryo-EM data.
- Macromolecular docking and sequence alignment.

Programming & Data Science:

- Languages: Python, C/C++, Bash, R (beginner).
- Machine Learning: Scikit-learn, TensorFlow.
- Workflow Management: Nextflow, Snakemake.
- Version Control: Git (Gitlab, Github).

6 Grants and Awards

- **2023** EMBO Childcare Grant
- **2022** SONATA 17 Grant (691,252 PLN), National Science Centre, Poland
- **2019** Poster Award, The RNA Society Meeting, Krakow, Poland
- **2019** Travel Fellowship, The RNA Society Meeting, Krakow, Poland
- **2012, 2014** Junior/Senior Research Fellowship, CSIR-UGC, India

7 Oral Presentations

- “Integrated modeling of RNA 3D structures with SimRNA-Cry,” EMBO Sectorial Meeting, Würzburg, Germany, April 2025.
- “Modeling 3D structure of RNA using low resolution cryo-EM maps with SimRNA-Cry,” EMBO Workshop, Heidelberg, Germany, December 2023.
- “SimRNA-Cry: a tool for modeling of RNA molecules using maps from cryo-electron microscopy,” Polish Bioinformatics Society Symposium, Warsaw, Poland, September 2022.

8 Declaration

I hereby declare that the information provided is accurate and truthful to the best of my knowledge. I consent to the processing of my personal data for recruitment and conference purposes.

Sunandan Mukherjee

Warsaw, Poland