

SUMIT TARAFDER

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Research Interests

Topics 3D structure prediction, refinement or quality estimation of protein, RNA and associated complexes.
Areas Structural bioinformatics, deep learning

Education

Virginia Tech

Ph.D. student in Computer Science

Aug. 2022 – Present

Blacksburg, VA

Bangladesh University of Engineering & Technology (BUET)

M.Sc. in Computer Science and Engineering

Jan. 2022

Dhaka, Bangladesh

Bangladesh University of Engineering & Technology (BUET)

B.Sc. in Computer Science and Engineering

Feb. 2017

Dhaka, Bangladesh

Experience

Virginia Tech

Graduate Research Assistant, Bhattacharya Lab

Aug. 2022 – Present

Blacksburg, VA

- Focused on projects related to the prediction and quality estimation of RNA 3D structures and protein-RNA complexes.
- Recently implemented research projects are available in *GitHub*.

Virginia Tech

Graduate Teaching Assistant

Aug. 2022 – Dec. 2022

Blacksburg, VA

- **CS 5914 TS: Warehouse Scale Computing (Fall 2022)**
 - * Graded multiple paper review and summary writings for individual students and conducted office hours.
- **CS 5805 Advanced Machine Learning (Fall 2025)**
 - * Responsible for assignment design & grading, project proposal & report evaluation (in-class sessions).

United International University

Lecturer, Department of Computer Science and Engineering

May 2017 – Oct. 2021

Dhaka, Bangladesh

- I was the instructor and coordinator for a wide range of undergraduate-level theory and practical courses.

Publications

- **Sumit Tarafder**, Debswapna Bhattacharya. “*PARSEbp: Pairwise Agreement-based RNA Scoring with Emphasis on Base Pairings*”, **2025**. [Under Review]
- **Sumit Tarafder**, Debswapna Bhattacharya. “*RNAbpFlow: Base pair-augmented SE(3)-flow matching for conditional RNA 3D structure generation*”, **2025**. [Under Review]
- **Sumit Tarafder**, Debswapna Bhattacharya. “*lociPARSE: a locality-aware invariant point attention model for scoring RNA 3D structures*”, Journal of Chemical Information and Modeling, Volume 64, Issue 22, Pages 8655–8664, **November 2024**. Impact Factor: 5.7
- **Sumit Tarafder**, Rahmatullah Roche, Debswapna Bhattacharya. “*The landscape of RNA 3D structure modeling with transformer networks*”, Biology Methods and Protocols, Volume 9, Page 47, Issue 1, **July 2024**. Impact Factor: 2.5
- **Sumit Tarafder**, Xinyu Wang, Rahmatullah Roche, Debswapna Bhattacharya. “*Advances in Language-Model-Informed Protein–Nucleic Acid Binding Site Prediction*”, Methods in Molecular Biology, Page 139-151, **July 2025**. Impact Factor: 1.3
- **Sumit Tarafder**, Mazharul Islam, Swakkhar Shatabda, Atif Rahman. “*Figbird: A probabilistic method for filling gaps in genome assemblies*”, Bioinformatics, Volume 38, **August 2022**, Pages 3717–3724, Issue 15. Impact factor: 6.9
- **Sumit Tarafder**, Md. Toukir Ahmed, Sumaiya Iqbal, Md Tamjidul Hoque, M. Sohel Rahman. “*RBSURFpred : Modeling Protein Accessible Surface Area in Real and Binary Space using Regularized and Optimized Regression*”, Journal of Theoretical Biology, Volume 441, **January 2018**, Pages 44 - 57. Impact factor: 2.0
- Rahmatullah Roche, **Sumit Tarafder**, Debswapna Bhattacharya. “*Single-sequence protein-RNA complex structure prediction by geometric attention-enabled pairing of biological language models*”, Cell Systems, **2025**. IF: 7.7.
- Rahmatullah Roche, Bernard Moussad, Md Hossain Shuvo, **Sumit Tarafder**, Debswapna Bhattacharya. “*EquiPNAS: improved protein-nucleic acid binding site prediction using protein-language-model-informed equivariant deep graph neural networks*”, NAR, volume 52, Page e27, Issue 5, **January 2024**. Impact Factor: 14.9

Talks

- Presented our work “*lociPARSE*” as a *poster* at *ISMB '24* (Montreal, CA).
- Presented “*lociPARSE*” as a full-length talk at *GLBIO conference* (Minnestota, USA).

Awards

Pratt Fellowship	Department of Computer Science, Virginia Tech. Awarded in <i>2024</i> and <i>2025</i> .
Travel Grant	Department of Computer Science, Virginia Tech. Supported participation at <i>ISMB 2024</i> .
Travel Grant	ISCB and GLBC. Supported presentation at <i>GLBIO 2025</i> .
Dean’s List Award	University Merit Scholarship and Dean’s List from (<i>BUET</i>).

Services

- Reviewer at IEEE/ACM Transactions on Computational Biology and Bioinformatics.
- Sub-reviewer at ISMB 2025, IEE BIBM 2025, IEE BIBM 2024, BIODDD 2024.

Skills

Languages: Python, Java, C, C++, HTML/CSS

Tools: Git, Docker, Chimera, PyMOL, VS Code

Frameworks: PyTorch, PyTorch Lightning, Matplotlib, Scikit-learn, LangChain