

# Parth Bibekar

## Curriculum Vitae

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### Education

- 2024–Present **Institute of Bioengineering, SV, EPFL, Switzerland,**  
*PhD candidate in Computational and Quantitative Biology.*  
Advisor: Prof. Matteo Dal Peraro
- 2019–2024 **Indian Institute of Science Education and Research, Kolkata, India,**  
*BSMS Dual Degree, Major in Biology & minor in Computational and Data Sciences.*  
CGPA – 8.21/10

### Research Interests

Research Int. Machine Learning for RNA design, Protein design and Molecular modeling

### Current Position

- Sept 2024– Ongoing I am a PhD student at the [Laboratory for Biomolecular modeling](#) at EPFL, Switzerland, under the supervision of Prof. Matteo Dal Peraro. Developing ML based techniques for various applications in biomolecular modeling, with a particular focus on RNA design and modeling protein-nucleotide complexes.

### Work Experience

- May 2022 – **Research Intern, EPFL, Switzerland,**  
Aug 2022 *with Prof. Matteo Dal Peraro at the Laboratory for Biomolecular Modeling.*
- Jun 2021 – **Research Intern, IISER Kolkata, India,**  
Jan 2023 *with Prof. Neelanjana Sengupta at (bio)molecular Computations: Energetics and Dynamics group.*

### Publications

- Jun 2025 Bibekar et al., Context-aware geometric deep learning for RNA sequence design. NeurIPS 2025 AI4D3 Workshop (2025), [10.1101/2025.06.21.660801](#)
- Apr 2024 Bibekar et al., PeSTo-Carbs: Geometric Deep Learning for Prediction of Protein-Carbohydrate Binding Interfaces. Journal of Chemical Theory and Computation (2024), [10.1021/acs.jctc.3c01145](#)
- Feb 2023 Dutta et al., Conformational ensemble of the NSP1 CTD in SARS-CoV-2: Perspectives from the free energy landscape, Biophysical Journal (2023), [10.1016/j.bpj.2023.02.010](#)

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## Achievements

Aug 2023 **E3 Program Fellow.**

- I was awarded the EPFL Excellence in Engineering Program fellowship, for a summer project in the Laboratory for Biomolecular Modeling at EPFL, Switzerland.

Jun 2022 **ThinkSwiss Research Scholarship.**

- I was awarded the ThinkSwiss Research Scholarship of for a period of three months for a research project in École polytechnique fédérale de Lausanne, Switzerland.

Dec 2021 **National HPC Hackathon.**

- Part of the winning team in the National HPC Hackathon organised by Amazon Web Services and Intel in association with the Office of Principal Scientific Advisor to the Government of India.

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## Projects

Sept 2024 – **Rlbonucleic acid Sequence design from TerTiary structure (RISoTTo), EPFL Lau-**  
Ongoing *sanne, Switzerland. DOI:*[10.1101/2025.06.21.660801](https://doi.org/10.1101/2025.06.21.660801).

- Developed RISoTTo, pioneering context-aware RNA sequence design by considering surrounding proteins, ligands, or ions.

June 2022 – **Predicting Protein - Carbohydrate binding interfaces using Deep Learning, Prof.**  
Sept 2024 *Matteo Dal Peraro, EPFL Lausanne, Switzerland, DOI:* [10.1021/acs.jctc.3c01145](https://doi.org/10.1021/acs.jctc.3c01145).

- Predicting binding interfaces between Proteins and Carbohydrates using deep geometric transformers.

Nov 2021–Oct 2022 **Exploring the the Free Energy Landscape of IDRs using Machine Learning, Prof.**  
*Neelanjana Sengupta, IISER Kolkata, India. DOI:*[10.1016/j.bpj.2023.02.010](https://doi.org/10.1016/j.bpj.2023.02.010).

- Study the Conformational Landscape of two SARS-CoV-2 IDRs using Molecular Dynamics Simulation and fitting FEL using GMM based models.
- Sample the intermediate rare Conformations using the data driven latent space

June 2021 – **Exploring the Free Energy Landscape of amyloid assembly, Prof. Neelanjana Sengupta,**  
Sept 2021 *IISER Kolkata, India.*

- Study the Free Energy Landscape of hIAPP fibril dissociation using Molecular Dynamics Simulations and enhance sampling methods.

Apr 2021 **WeLearn Bot** [\[Code\]](#), *Team Project.*

- I created and maintain a cli application for interacting with WeLearn in the IISER-Kolkata domain.
- The application is widely used by many students in IISER Kolkata and has been released as a Python package.

Find my other projects here [🔗 Github: ParthBibekar](#).

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## Teaching Experience

2025 **TA BIOENG-455: Computational Cell Biology.**

- Supervised students for various aspects of the course.

2024 **TA BIO-315: Structural biology.**

- Supervised students for modules: Molecular Dynamics, Molecular Modeling and CryoEM analysis.

## Conferences

- Dec 2025 NeurIPS AI4D3 Workshop (**Poster**), San Diego, USA
- Oct 2025 European RosettaCon (**Poster**), Ljubljana, Slovenia
- Oct 2025 Structure Based Drug Discovery (**Poster**), Sestri Levante, Italy
- Nov 2024 European RosettaCon (**Poster**), Copenhagen, Denmark

## Skills

- Languages Python, C, MATLAB, Bash
- Frameworks TensorFlow, Keras, PyTorch, PyTorch Geometric
- Molecular Dynamics GROMACS, AMBER, PLUMED
- HPC AWS, GCC, etc.
- Data analysis Gnuplot, OriginLab
- Utilities Conda/Anaconda, Git/Github, VScode, Jupyter Notebook
- Web Dev HTML/CSS