Parth Bibekar

Curriculum Vitae

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Education

Sept 2024– Ongoing — **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 – Aug 2022 — **Research Intern, EPFL, Switzerland**,
with Prof. Matteo Dal Peraro at the Laboratory for Biomolecular Modeling.

Jun 2021 – Jan 2023 — **Research Intern, IISER Kolkata, India**,
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. Jounal 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

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.

Projects

Sept 2024 – Ongoing **RIbonucleic acid Sequence design from TerTiary structure (RISoTTo)**, *EPFL Lausanne, Switzerland. DOI:10.1101/2025.06.21.660801*.
- Developed RISoTTo, pioneering context-aware RNA sequence design by considering surrounding proteins, ligands, or ions.

June 2022 – Sept 2024 **Predicting Protein - Carbohydrate binding interfaces using Deep Learning**, *Prof. Matteo Dal Peraro, EPFL Lausanne, Switzerland, DOI: 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*.
- 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 – Sept 2021 **Exploring the Free Energy Landscape of amyloid assembly**, *Prof. Neelanjana Sengupta, IISER Kolkata, India*.
- Study the Free Energy Landscape of hIAPP fibril dissociation using Molecular Dynamics Simulations and enchance 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.

Teaching Experience

2025 **TA BIOENG-455: Computational Cell Biology**.
- Supervised students for various aspects of the course.

2024, 2026 **TA BIO-315: Structural biology**.
- Supervised students for modules: Molecular Dynamics, Molecular Modeling and CryoEM analysis.

Conferences & Invited Talks

Jan 2026	EPFL AIxBIO seminar (**Talk**), EPFL, Switzerland
Jan 2026	Swiss RNA Workshop (**Poster**), Bern, Switzerland
Jan 2026	frontiers2026 symposium on NanoBioEngineering (**Talk**), EPFL, Switzerland
Jan 2026	SIB AI4Biomolecules SIG seminar (**Talk**), Bern, Switzerland
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