Rajarshi SinhaRoy

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LinkedIn | GitHub | Google Scholar

Research Profile

PhD researcher in Informatics at the University of Leipzig (Germany), specializing in Artificial Intelligence for Drug Discovery. My research integrates deep learning, bioinformatics, and structural biology to design interpretable models that predict enzyme function, protein stability, and structure–function relationships. With expertise in geometric deep learning, molecular simulation, and biomolecular modeling, I aim to bridge algorithmic innovation and molecular biophysics for predictive, explainable discovery of therapeutic enzymes and drug targets.

Education

PhD in Informatics
Institute of Drug Discovery, University of Leipzig, Germany *Nov 2023 – Present*

Focus: AI for mRNA delivery, Geometric Deep Learning, Protein Modeling, Brownian Dynamics, Molecular Dynamics and Computational Biology.
Supervisors: Prof. Dr. Jens Meiler; Dr. Georg Künze.

M.Sc. in Computer Science
St. Xavier's College (Autonomous), Kolkata, India *2020 – 2022*

CGPA 8.36 • Dissertation: *Optimization in Image Processing and Deep Learning.*

B.Sc. in Computer Science
Government General Degree College, Singur, India *2017 – 2020*

CGPA 8.83 • Focus: Artificial Intelligence, Database Systems, Applied Computing.

Research & Professional Experience

PhD Researcher — Artificial Intelligence for Drug Discovery
University of Leipzig, Germany *Nov 2023 – Present*

- Collaborative project with **BioNTech** on enhancing mRNA delivery therapeutics through computational design.
- Developing **SE(3)-equivariant GNNs** for enzyme pH-optima prediction.
- Designing **MPNN–Transformer** architectures for pH-dependent protein sequence generation.
- Conducting molecular-dynamics simulations and bioinformatics analyses for interpretable AI models.

Academic Researcher — Bioinformatics and AI Lab
Kolkata, India *2021 – 2023*

- Designed hybrid **GAN + DCNN** architectures for MRI-based Alzheimer's progression prediction.
- Built preprocessing, augmentation, and evaluation pipelines ensuring reproducibility.

Teaching Assistant — Computer Science Department
Techno Main Salt Lake, India *Jan 2023 – Oct 2023*

- Assisted undergraduate courses in Computer Science and Data Analytics.
- Conducted lab tutorials and supervised ML/AI-based student projects.

Developer Intern — EasyWay Technologies
Kolkata, India *Jan 2022 – Apr 2022*

- Developed and deployed backend services (PHP, MySQL) and data visualization modules for a client-facing analytics platform.
- Implemented analytics automation and optimized API performance.

Software Developer Intern — Unique Start
Kolkata, India *May 2021 – Oct 2021*

- Developed REST APIs and front-end integrations for a scalable data platform.
- Improved scalability by optimizing SQL queries and adding a data caching layer, reducing API latency.

Publications & Conferences

Preprints

- R. SinhaRoy, C. Clauss, I. Ivanikov, and G. Künze, "Predicting Enzyme pH Optima from Structure Using Equivariant Graph Neural Networks," *bioRxiv*, 2026. doi:10.64898/2026.01.18.700076.

Peer-Reviewed Publications

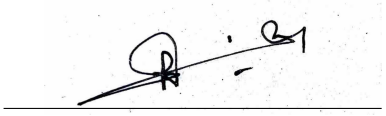
- R. SinhaRoy and A. Sen, "A Hybrid Deep Learning Framework to Predict Alzheimer's Disease Progression Using GAN and DCNN," *Arabian Journal for Science and Engineering*, 2023. doi:10.1007/s13369-023-07973-9.
- R. Sinharoy and A. Sen, "Cardiovascular Disease Prediction Using Ensemble Classification Algorithm in Machine Learning," *International Journal of Soft Computing*, 2022. doi:10.21917/ijsc.2022.0366.
- R. Sinharoy and S. Sarkhel, "Air Quality Index Prediction in Realtime Using SVM," *International Journal of Innovative Research in Physics*, 2021. doi:10.15864/ijiip.3106.
- R. SinhaRoy, "A Study on the Journey of NLP Models: From Symbolic NLP to BERT," *IJSRCSEIT*, 2021. doi:10.32628/CSEIT217688.

Conference Presentations

- R. SinhaRoy, "pHoptNN: Predicting Enzyme *pH*-Optima from Structure Using Equivariant Graph Neural Networks," Oral Presentation, *EUROSETTACON 2025*.
- S. Sen, S. Sonali, R. SinhaRoy et al., "Overlapped Fingerprint Separation Using Graph-Based Model," in *IEEE Silchar Subsection Conference (SILCON)*, 2022. doi:10.1109/SILCON55242.2022.10028828.

Technical Skills

Programming: Python • C/C++ • Java • SQL • MATLAB • PHP • HTML/CSS/JS • Git
ML/DL: TensorFlow • Keras • PyTorch • GNNs • CNNs • GANs • MPNNs • Diffusion Models
Bio-Software: RFDiffusion • ProteinMPNN • GROMACS • AMBER • VMD • AlphaFold • PyMOL
Research Areas: Computational Biology • Bioinformatics • Data Mining • Molecular Dynamics



May 20, 2026
Leipzig, DE

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