Rajarshi Roy

Ph.D. in Computational Biophysics • Postdoctoral Research Associate, Purdue University

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RESEARCH INTERESTS

Computational biophysics; all-atom and enhanced-sampling molecular dynamics; conformational path sampling and structural transitions in proteins; kinase regulation and dynamics; effects of post-translational modifications on protein structure; protein–carbohydrate interactions; free energy calculations and structure-based drug discovery.

EDUCATION

Ph.D., Biosciences and Biomedical Engineering (Computational Biophysics) 2017 – 2022
Indian Institute of Technology Indore *Madhya Pradesh, India*
Thesis: Glycans in-silico — Investigating Conformational Dynamics and Interactions with Proteins. Advisor: Dr. Parimal Kar.

M.Sc., Biophysics 2014 – 2016
University of Kalyani *West Bengal, India*
Dissertation: Asymmetry of Perceptual Filling-In of the Blind Spot. Advisor: Dr. Kuntal Ghosh (Indian Statistical Institute).

B.Sc., Physics (Honors) 2011 – 2014
University of Calcutta *West Bengal, India*

RESEARCH EXPERIENCE

Postdoctoral Research Associate Aug 2022 – Present
Purdue University, Dept. of Medicinal Chemistry & Molecular Pharmacology — Advisor: Prof. Carol Beth Post West Lafayette, IN

- Research on conformational path sampling strategies in protein structures, simulating kinase dynamics, and assessing the effects of post-translational modifications on structure.
- Multi-microsecond all-atom MD simulations of the Focal Adhesion Kinase (FAK) kinase–FERM complex across phosphorylation states on the Anton2 specialized supercomputer.
- Development of the Adaptive Biasing Path Optimization (ABPO) method for characterizing structural transitions between protein conformations (CHARMM Fortran and Python/OpenMM GPU implementations).

Doctoral Researcher 2017 – 2022
Indian Institute of Technology Indore — Advisor: Dr. Parimal Kar *Indore, India*

- Computational analysis of glycan molecules, including extensive sampling of diverse glycan structures and detailed examination of protein–glycan interactions and binding affinities.
- Enhanced sampling (Gaussian accelerated MD, REMD) and free energy calculations across glycan, viral protein, and drug-target systems.

Trainee 2016
Indian Statistical Institute — Advisor: Dr. Kuntal Ghosh *Kolkata, India*

- Investigated perceptual blind-spot filling-in with various stimuli; implemented MATLAB-based analysis of psychophysical studies.

TEACHING EXPERIENCE

Invited Instructor — Workshop on Molecular Docking & MD Simulations Dec 2024
Woxsen University, School of Sciences (invited by Dept. of Biotechnology) *Hyderabad, India*

- Delivered a two-day hands-on workshop (Dec 16–17, 2024) introducing molecular docking and MD simulation fundamentals to PG students, Ph.D. scholars, postdoctoral researchers, and early-career faculty, with practical training in AutoDock Vina and GROMACS for drug discovery and biomolecular analysis.

Graduate Teaching Assistant — Bioinformatics: Theory & Laboratory (BSE 618) 2018 – 2020
Indian Institute of Technology Indore, Dept. of Biosciences and Biomedical Engineering *Indore, India*

- Three semesters of teaching assistantship for postgraduate students in the Bioinformatics: Theory and Laboratory course.

PUBLICATIONS

30 peer-reviewed journal articles (# denotes equal contribution). h-index and citation metrics available on Google Scholar.

Peer-Reviewed Journal Articles

1. Kashyap, D., Koirala, S., **Roy, R.**, Saini, V., Varshney, N., Bagde, P.H., Samanta, S., Kar, P. and Jha, H.C., Computational insights into VacA toxin inhibition: harnessing FDA-approved antibiotics against Helicobacter pylori. *Journal of Biomolecular Structure and Dynamics, 42(24), 13725–13737 (2024).*
2. Poddar, S., **Roy, R.** and Kar, P., Elucidating the conformational dynamics of histo-blood group antigens and their interactions with the rotavirus spike protein through a computational lens. *Journal of Biomolecular Structure and Dynamics, 42(23), 13201–13215 (2024).*
3. Kashyap, D., **Roy, R.**, Varshney, N., Baral, B., Bagde, P.H., Kandpal, M., Kumar, S., Kar, P. and Jha, H.C., Withania somnifera extract reduces gastric cancerous properties through inhibition of gankyrin in cellular milieu produced by Helicobacter pylori and Epstein Barr virus. *Journal of Biomolecular Structure and Dynamics, 42(18), 9399–9415 (2024).*
4. Koirala, S.#, **Roy, R.#**, Samanta, S., Mahapatra, S. and Kar, P., Plant-derived active compounds of ayurvedic neurological formulation Saraswatharishta as a potential dual leucine zipper kinase inhibitor: an in-silico study. *Journal of Biomolecular Structure and Dynamics, 42(20), 11201–11214 (2024).*
5. Mukherjee, A., Paul, A., **Roy, R.** and Ghosh, K., The role of extrinsic and intrinsic factors in perceptual filling-in of the blind-spot with variegated color and texture stimuli. *Vision Research, 222, 108452 (2024).*
6. Are, V.N., **Roy, R.**, Dhanda, S.K., Neema, S., Sahu, N.R., Adithya, N., Tiwari, R., Kar, P. and Nayak, D., Predicting immune response targets in orthoflaviviruses through sequence homology and computational analysis. *Journal of Molecular Modeling, 30(8), 295 (2024).*
7. Poddar, S., **Roy, R.** and Kar, P., The conformational dynamics of Hepatitis C Virus E2 glycoprotein with the increasing number of N-glycosylation unraveled by molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics, 1–16 (2024).*
8. Singh, S., Ghosh, P., **Roy, R.**, Behera, A., Sahadevan, R., Kar, P., Sadhukhan, S. and Sonawane, A., 4″-Alkyl EGCG derivatives induce cytoprotective autophagy response by inhibiting EGFR in glioblastoma cells. *ACS Omega, 9(2), 2286–2301 (2024).*
9. Jaiswal, A., **Roy, R.**, Tamrakar, A., Singh, A.K., Kar, P. and Kodgire, P., Activation-induced cytidine deaminase, an antibody diversification enzyme, interacts with chromatin modifier UBN1 in B-cells. *Scientific Reports, 13(1), 19615 (2023).*
10. **Roy, R.**, Sk, M.F., Tanwar, O. and Kar, P., Computational studies indicated the effectiveness of human metabolites against SARS-CoV-2 main protease. *Molecular Diversity, 27(4), 1587–1602 (2023).*
11. Kashyap, D.#, **Roy, R.#**, Kar, P. and Jha, H.C., Plant-derived active compounds as a potential nucleocapsid protein inhibitor of SARS-CoV-2: an in-silico study. *Journal of Biomolecular Structure and Dynamics, 41(10), 4770–4785 (2023).*
12. **Roy, R.**, Poddar, S., Sk, M.F. and Kar, P., Conformational preferences of triantennary and tetraantennary hybrid N-glycans in aqueous solution: insights from 20 μs long atomistic molecular dynamic simulations. *Journal of Biomolecular Structure and Dynamics, 41(8), 3305–3320 (2023).*
13. **Roy, R.**, Poddar, S. and Kar, P., Comparison of the conformational dynamics of an N-glycan in implicit and explicit solvents. *Carbohydrate Research, 522, 108700 (2022).*

14. **Roy, R.**, Sk, M.F., Jonniya, N.A., Poddar, S. and Kar, P., Finding potent inhibitors against SARS-CoV-2 main protease through virtual screening, ADMET, and molecular dynamics simulation studies. *Journal of Biomolecular Structure and Dynamics, 40(14), 6556–6568 (2022).*
15. Rehman, S., Bishnoi, S., **Roy, R.**, Kumari, A., Jayakumar, H., Gupta, S., Kar, P., Pattnaik, A.K. and Nayak, D., Emerging biomedical applications of the vesicular stomatitis virus glycoprotein. *ACS Omega, 7(37), 32840–32848 (2022).*
16. Jaiswal, S., **Roy, R.**, Dutta, S.B., Bishnoi, S., Kar, P., Joshi, A., Nayak, D. and Gupta, S., Role of doxorubicin on the loading efficiency of ICG within silk fibroin nanoparticles. *ACS Biomaterials Science & Engineering, 8(7), 3054–3065 (2022).*
17. **Roy, R.**, Jonniya, N.A. and Kar, P., Effect of sulfation on the conformational dynamics of dermatan sulfate glycosaminoglycan: a Gaussian accelerated molecular dynamics study. *The Journal of Physical Chemistry B, 126(21), 3852–3866 (2022).*
18. **Roy, R.**, Jonniya, N.A., Sk, M.F. and Kar, P., Comparative structural dynamics of isoforms of Helicobacter pylori adhesin BabA bound to Lewis b hexasaccharide via multiple-replica molecular dynamics simulations. *Frontiers in Molecular Biosciences, 9, 852895 (2022).*
19. Sk, M.F., Jonniya, N.A., **Roy, R.** and Kar, P., Phosphorylation-induced conformational dynamics and inhibition of Janus Kinase 1 by suppressors of cytokine signaling 1. *The Journal of Physical Chemistry B, 126(17), 3224–3239 (2022).*
20. **Roy, R.#**, Mishra, A.#, Poddar, S., Nayak, D. and Kar, P., Investigating the mechanism of recognition and structural dynamics of nucleoprotein–RNA complex from Peste des petits ruminants virus via Gaussian accelerated molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics, 40(5), 2302–2315 (2022).*
21. Sk, M.F., Jonniya, N.A., **Roy, R.** and Kar, P., Unraveling the molecular mechanism of recognition of selected next-generation antirheumatoid arthritis inhibitors by Janus kinase 1. *ACS Omega, 7(7), 6195–6209 (2022).*
22. Jonniya, N.A., Sk, M.F., **Roy, R.** and Kar, P., Discovery of potential competitive inhibitors against With-No-Lysine kinase 1 for treating hypertension by virtual screening, inverse pharmacophore-based lead optimization, and molecular dynamics simulations. *SAR and QSAR in Environmental Research, 33(2), 63–87 (2022).*
23. Singh, S., Sahadevan, R., **Roy, R.**, Biswas, M., Ghosh, P., Kar, P., Sonawane, A. and Sadhukhan, S., Structure-based design and synthesis of a novel long-chain 4″-alkyl ether derivative of EGCG as a potent EGFR inhibitor: in vitro and in silico studies. *RSC Advances, 12(28), 17821–17836 (2022).*
24. **Roy, R.**, Jonniya, N.A., Poddar, S., Sk, M.F. and Kar, P., Unraveling the molecular mechanism of recognition of human interferon-stimulated gene product 15 by coronavirus papain-like proteases: a multiscale simulation study. *Journal of Chemical Information and Modeling, 61(12), 6038–6052 (2021).*
25. Sk, M.F., Haridev, S., **Roy, R.** and Kar, P., Investigating potency of TMC-126 against wild-type and mutant variants of HIV-1 protease: a molecular dynamics and free energy study. *SAR and QSAR in Environmental Research, 32(11), 941–962 (2021).*
26. Sk, M.F., **Roy, R.**, Jonniya, N.A., Poddar, S. and Kar, P., Elucidating the biophysical basis of binding of inhibitors to SARS-CoV-2 main protease by using molecular dynamics simulations and free energy calculations. *Journal of Biomolecular Structure and Dynamics, 39(10), 3649–3661 (2021).*
27. Sk, M.F., **Roy, R.** and Kar, P., Exploring the potency of currently used drugs against HIV-1 protease of subtype D variant by using multiscale simulations. *Journal of Biomolecular Structure and Dynamics, 39(3), 988–1003 (2021).*
28. Thurakkal, L., Singh, S., **Roy, R.**, Kar, P., Sadhukhan, S. and Porel, M., An in-silico study on selected organosulfur compounds as potential drugs for SARS-CoV-2 infection via binding multiple drug targets. *Chemical Physics Letters, 763, 138193 (2021).*
29. Sk, M.F., Jonniya, N.A., **Roy, R.**, Poddar, S. and Kar, P., Computational investigation of structural dynamics of SARS-CoV-2 methyltransferase-stimulatory factor heterodimer nsp16/nsp10 bound to the cofactor SAM. *Frontiers in Molecular Biosciences, 7, 590165 (2020).*
30. **Roy, R.**, Ghosh, B. and Kar, P., Investigating conformational dynamics of Lewis Y oligosaccharides and elucidating blood group dependency of cholera using molecular dynamics. *ACS Omega, 5(8), 3932–3942 (2020).*

Conference Proceedings

1. Mukherjee, A., Paul, A., **Roy, R.**, Roy, S. and Ghosh, K. Perceptual filling-in of blind-spot for surrounding color gradient stimuli. *International Conference on Intelligent Human Computer Interaction, 194–204. Springer, Cham (2018).*

CONFERENCE PRESENTATIONS

1. Comprehensive Study of Structural Transitions Between Protein Conformations via Adaptively Biased Path Optimization.
   39th Annual Symposium of The Protein Society, San Francisco, CA, June 26–29, 2025. [Oral & Poster]
2. Exploring Phosphorylation-Driven Interdomain Dynamics Between FAK's Kinase and FERM Domains Through Molecular Dynamics.
   ACS Fall 2024, Denver, CO, August 18–22, 2024. [Oral]
3. Consequences of Multisite Phosphorylation on the Structure of Focal Adhesion Kinase.
   SCBB/SBBC Grad/Postdoc Symposium, Purdue University, December 13, 2023. [Oral]
4. Investigating Thermodynamics of Protein Structure with Multiscale Simulation and Machine Learning.
   Purdue Institute for Drug Discovery 8th Annual Symposium, Purdue University, October 6, 2023. [Poster]
5. Investigating the Conformational Landscapes of FabH and Src Kinase Using All-Atom Molecular Dynamics Simulations.
   Hitchhiker's Guide to the Biomolecular Galaxy 2023, Purdue University, May 16–17, 2023. [Poster]
6. Effect of Sulfation on the Conformational Dynamics of Dermatan Sulfate Glycosaminoglycan: A Gaussian Accelerated Molecular Dynamics Study.
   44th Indian Biophysical Society Meeting, ACTREC, India (online), March 30–April 1, 2022. [Poster]
7. Spatiotemporal Characterisations of Dermatan Sulphate Glycosaminoglycan Chains Through Enhanced Sampling.
   8th Annual Research Symposium, Centre for BioSystem Science and Engineering, Indian Institute of Science (online), January 28–29, 2022. [Poster]
8. Conformational Preferences of Tri-antennary and Tetra-antennary Hybrid N-glycans in Aqueous Solution: Insights from 20 μs Long Atomistic Molecular Dynamic Simulations.
   Physical Chemistry Physical Biology (PCPB) (online), September 24–28, 2021. [Oral]
9. Structural Dynamics and Recognition of Lewis Y Oligosaccharides by Cholera Toxin: A Molecular Dynamics and Free Energy Study.
   Computational Biology and Bioinformatics (CBB-2019), IIT Jodhpur, July 31–August 1, 2019. [Poster]
10. Investigating Conformational Flexibility of N-Glycans via All-Atom Molecular Dynamics Simulations.
    International Conference on Mathematical Modelling and Scientific Computing (ICMMSC-2018), IIT Indore, July 19–21, 2018. [Poster]
11. Elucidating Energetic Basis of Differential Binding Affinity of GRL-10413 Against HIV-1 and HIV-2 Protease and Mutation-Induced Changes in Binding Affinity Against HIV-1 Protease.
    International Conference on Emerging Area in Biosciences and Biomedical Technologies-1 (ebbt-1), IIT Indore, July 5–6, 2018. [Poster]
12. Molecular Recognition of Drugs by Receptor Proteins via Multiscale Simulation Methods.
    5th Industry Academia Conclave (IAC), IIT Indore, September 6, 2017. [Poster]

MENTORING

M.Sc. Dissertation Students (at IIT Indore)

- Naveen Kumar — Molecular Interaction Between Typhoid Toxin and N-linked Glycans: an in-silico Investigation (Jun 2021 – Jun 2022).
- Rohit Kumar Singh — Targeting SARS-CoV-2 Spike Protein with Human Metabolites: an in-silico Study for Drug Development (Jun 2020 – Jun 2021).
- Nima Tshering Bhutia — Drug Binding Analysis Against a Novel Target in Tuberculosis: a Molecular Dynamics Approach (Dec 2017 – Dec 2018).

Summer Trainees (at IIT Indore)

- Purushottam Behera (NIT Rourkela), Jyotirmoy Behera (NIT Rourkela), Yuvraj Rallapalli (Manipal Institute) — In-silico Investigation of Kinase Inhibitors Against FMS-like Tyrosine Kinase-3 (Jun–Aug 2021).
- Prarthita Rakshit (NIT Durgapur), Hari Om (NIT Durgapur) — Understanding the Recognition Mechanism Between Typhoid Toxin and Glycans (Jun–Aug 2021).

GRANTS & AWARDS

- Principal Investigator — Grant from the Center for Indian Scientific Knowledge Systems (CISKS), IIT Indore. Project: In-Silico Systematic Study of Ayurvedic Neuroprotective Herbs Against Dual Leucine Zipper Kinase for the Treatment of Neurodegeneration (9 months).
- Graduate Aptitude Test in Engineering (GATE) 2017 — All-India Rank 153.

PROFESSIONAL SERVICE

Journal Peer Review

- Reviewer — Communications Biology; Frontiers in Molecular Biosciences; Journal of Biomolecular Structure and Dynamics; Computers in Biology and Medicine.

Conference Organization (Volunteer)

- International Conference on Emerging Area in Biosciences and Biomedical Technologies-2 (ebbt-2), February 7–9, 2020.
- International Conference on Mathematical Modelling and Scientific Computing (ICMMSC-2018), July 19–21, 2018.
- International Conference on Emerging Area in Biosciences and Biomedical Technologies-1 (ebbt-1), January 5–6, 2018.

WORKSHOPS & TRAINING

- Summer School on Machine Learning in Bioinformatics, HSE University, Moscow, Russia (online), June 14–16, 2021.
- Simulation Methods in Scientific Computing, NSM Nodal Centre on HPC & AI, IIT Kharagpur (online), August 23–27, 2021.
- Computational Approaches in Drug Design & Therapeutics, Amity Institute of Biotechnology, Amity University Chhattisgarh (online), February 20, 2021.
- Computational Biology and Bioinformatics, IIT Jodhpur, July 31–August 1, 2021.
- Business Analytics using R, IIM Indore, March 20, 2019.
- Practical Protein Crystallography using PX Beamline at Indus-2 Synchrotron, RRCAT, March 27–28, 2018.
- In Silico Analysis of Mutation, University of Kalyani, December 16, 2015.

CERTIFICATIONS

- Building Transformer-Based Natural Language Processing Applications — NVIDIA Deep Learning Institute (2021).
- Fundamentals of Deep Learning — NVIDIA Deep Learning Institute (2021).
- Introduction to Computational Drug Design — Schrödinger & Pharmacy Council of India (2021).
- Nano-biotechnology in Drug Discovery, Development and Delivery — QIP, AICTE & IIT Indore (2021).
- Data Science and Analytics — NPIU/TEQIP-III & IIT Indore (2020).
- GPU Computing in Computational Biology — IIT Indore (2020).
- Introduction to Machine Learning — NPTEL & IIT Kharagpur (2016).

TECHNICAL SKILLS

Programming: Python, R, FORTRAN, Shell scripting, MATLAB, LaTeX

Simulation & Modeling: CHARMM, AMBER, GROMACS, NAMD, OpenMM, AutoDock, Schrödinger Suite

Analysis & Visualization: MDAnalysis, MDTraj, FreeSASA, cpptraj, UCSF Chimera/ChimeraX, PyMOL, VMD, Matplotlib

Methods: Enhanced sampling (gaMD, metadynamics, REMD, ABPO), free energy calculations (MM/PBSA, interaction energy decomposition), clustering, dimensionality reduction

Computing: Linux, HPC/SLURM, multi-node GPU clusters, Anton2, Git

Languages: Bengali (native), English (proficient), Hindi (conversational)