Rajarshi Roy

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*Exp*eriences

Purdue University
West Lafayette, US
Post Doc RESEARCH ASSOCIATE
2022-Present

- **Advisor:** Prof. Carol Beth Post
- **Area of Study:** My research focuses on estimating conformational path sampling strategies in protein structures, simulating kinase dynamics, and assessing post-translational modifications' (PTMs) effects on structure.

Indian Institute of Technology Indore
Indore, India
TEACHING ASSISTANTSHIP
2018-2020

- Three semesters of teaching assistantship of PG students for Bioinformatics: Theory and Laboratory course (BSE 618) of Biosciences and Biomedical Engineering

Indian Statistical Institute
Kolkata, India
TRAINEE
2016

- Investigated blind spot filling-in with various stimuli.
- Implemented MATLAB for psychophysical study analysis.

*Edu*cation

Indian Institute of Technology Indore
Madhya Pradesh, India
Ph.D. IN BIOSCIENCES AND BIOMEDICAL ENGINEERING (COMPUTATIONAL BIOPHYSICS)
2017-2022

- **Thesis Title:** Glycans *in-silico*: Investigating Conformational Dynamics and Interactions with Proteins
- **Advisor:** Dr. Parimal Kar
- **Area of Study:** computational analysis of glycan molecules, encompassing extensive sampling of diverse glycan structures, alongside a detailed examination of protein-glycan interactions and their binding affinities

University of Kalyani
West Bengal, India
M.Sc. IN BIOPHYSICS
2014-2016

- **Dissertation Title:** Asymmetry of Perceptual Filling-In of the Blind Spot
- **Advisor:** Dr. Kuntal Ghosh
- **Area of Study:** Psychophysics

University of Calcutta
West Bengal, India
B.Sc. IN PHYSICS (HONORS)
2011-2014

*Pub*lications

Peer-reviewed Journals: [#Equal Contribution]

1. Kashyap, D., Koirala, S., **Roy, R.**, Saini, V., Varshney, N., Bagde, P.H., Samanta, S., Kar, P. and Jha, H.C., **2024**. Computational insights into VacA toxin inhibition: harnessing FDA-approved antibiotics against Helicobacter pylori. *Journal of Biomolecular Structure and Dynamics*, *42*(24), pp.13725-13737.
   DOI: https://doi.org/10.1080/07391102.2023.2278080
2. Poddar, S., **Roy, R.** and Kar, P., **2024**. Elucidating the conformational dynamics of histo-blood group antigens and their interactions with the rotavirus spike protein through computational lens. *Journal of Biomolecular Structure and Dynamics*, *42*(23), pp.13201-13215.
   DOI: https://doi.org/10.1080/07391102.2023.2274979
3. Kashyap, D., **Roy, R.**, Varshney, N., Baral, B., Bagde, P.H., Kandpal, M., Kumar, S., Kar, P. and Jha, H.C., **2024**. 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), pp.9399-9415.
   DOI: https://doi.org/10.1080/07391102.2023.2252096
4. Koirala, S.[#], **Roy, R.**[#], Samanta, S., Mahapatra, S. and Kar, P., 2024. 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), pp.11201-11214.
   DOI: https://doi.org/10.1080/07391102.2023.2260892
5. Mukherjee, A., Paul, A., **Roy, R.** and Ghosh, K., **2024**. The role of extrinsic and intrinsic factors in perceptual filling-in of the blind-spot with variegated color and texture stimuli. *Vision Research*, *222*, p.108452.
   DOI: https://doi.org/10.1016/j.visres.2024.108452
6. Are, V.N., **Roy, R.**, Dhanda, S.K., Neema, S., Sahu, N.R., Adithya, N., Tiwari, R., Kar, P. and Nayak, D., **2024**. Predicting immune response targets in orthoflaviviruses through sequence homology and computational analysis. *Journal of Molecular Modeling*, *30*(8), p.295.
   DOI: https://doi.org/10.1007/s00894-024-06088-8
7. Poddar, S., **Roy, R.** and Kar, P., **2024**. 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*, pp.1-16.
   DOI: 10.1080/07391102.2024.2319679
8. Singh, S., Ghosh, P., **Roy, R.**, Behera, A., Sahadevan, R., Kar, P., Sadhukhan, S. and Sonawane, A., **2024**. 4 ″-Alkyl EGCG Derivatives Induce Cytoprotective Autophagy Response by Inhibiting EGFR in Glioblastoma Cells. *ACS omega*, *9*(2), pp.2286-2301.
   DOI: https://doi.org/10.1021/acsomega.3c06110
9. Jaiswal, A., **Roy, R.**, Tamrakar, A., Singh, A.K., Kar, P. and Kodgire, P., **2023**. Activation-induced cytidine deaminase an antibody diversification enzyme interacts with chromatin modifier UBN1 in B-cells. *Scientific Reports*, *13*(1), p.19615.
   DOI: https://doi.org/10.1038/s41598-023-46448-7
10. **Roy, R.**, Sk, M.F., Tanwar, O. and Kar, P., **2023**. Computational studies indicated the effectiveness of human metabolites against SARS-Cov-2 main protease. *Molecular Diversity*, *27*(4), pp.1587-1602.
    DOI: https://doi.org/10.1007/s11030-022-10513-6
11. Kashyap, D.[#], **Roy, R.**[#], Kar, P. and Jha, H.C., **2023**. 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), pp.4770-4785.
    DOI: https://doi.org/10.1080/07391102.2022.2072951

12. **Roy, R.**, Poddar, S., Sk, M.F. and Kar, P., **2023**. 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), pp.3305-3320.
DOI: https://doi.org/10.1080/07391102.2022.2047109
13. **Roy, R.**, Poddar, S. and Kar, P., **2022**. Comparison of the conformational dynamics of an N-glycan in implicit and explicit solvents. *Carbohydrate Research*, *522*, p.108700.
DOI: https://doi.org/10.1016/j.carres.2022.108700
14. **Roy, R.**, Sk, M.F., Jonniya, N.A., Poddar, S. and Kar, P., **2022**. 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), pp.6556-6568.
DOI: https://doi.org/10.1080/07391102.2021.1897680
15. Rehman, S., Bishnoi, S., **Roy, R.**, Kumari, A., Jayakumar, H., Gupta, S., Kar, P., Pattnaik, A.K. and Nayak, D., **2022**. Emerging biomedical applications of the vesicular stomatitis virus glycoprotein. *ACS omega*, *7*(37), pp.32840-32848.
DOI: https://doi.org/10.1021/acsomega.2c03517
16. Jaiswal, S., **Roy, R.**, Dutta, S.B., Bishnoi, S., Kar, P., Joshi, A., Nayak, D. and Gupta, S., **2022**. Role of doxorubicin on the loading efficiency of ICG within silk fibroin nanoparticles. *ACS Biomaterials Science & Engineering*, *8*(7), pp.3054-3065.
DOI: https://doi.org/10.1021/acsbiomaterials.1c01616
17. **Roy, R.**, Jonniya, N.A. and Kar, P., **2022**. 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), pp.3852-3866.
DOI: https://doi.org/10.1021/acs.jpcb.2c01807
18. **Roy, R.**, Jonniya, N.A., Sk, M.F. and Kar, P., **2022**. 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*, p.852895.
DOI: https://doi.org/10.3389/fmolb.2022.852895
19. Sk, M.F., Jonniya, N.A., **Roy, R.** and Kar, P., **2022**. Phosphorylation-induced conformational dynamics and inhibition of Janus Kinase 1 by suppressors of cytokine signaling 1. *The Journal of Physical Chemistry B*, *126*(17), pp.3224-3239.
DOI: https://doi.org/10.1021/acs.jpcb.1c10733
20. **Roy, R.**[#], Mishra, A.[#], Poddar, S., Nayak, D. and Kar, P., **2022**. 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), pp.2302-2315.
DOI: https://doi.org/10.1080/07391102.2020.1838327
21. Sk, M.F., Jonniya, N.A., **Roy, R.** and Kar, P., **2022**. Unraveling the molecular mechanism of recognition of selected next-generation antirheumatoid arthritis inhibitors by Janus kinase 1. *ACS omega*, *7*(7), pp.6195-6209.
DOI: https://doi.org/10.1021/acsomega.1c06715
22. Jonniya, N.A., Sk, M.F., **Roy, R.** and Kar, P., **2022**. 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), pp.63-87.
DOI: https://doi.org/10.1080/1062936X.2021.2023218
23. Singh, S., Sahadevan, R.**, Roy**, **R.**, Biswas, M., Ghosh, P., Kar, P., Sonawane, A. and Sadhukhan, S., **2022**. Structure-based design and synthesis of a novel long-chain 4′′-alkyl ether derivative of EGCG as potent EGFR inhibitor: In vitro and in silico studies. *RSC advances*, *12*(28), pp.17821-17836.
DOI: https://doi.org/10.1039/D2RA01919A

24. **Roy, R.**, Jonniya, N.A., Poddar, S., Sk, M.F. and Kar, P., **2021**. 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), pp.6038-6052. **DOI:** https://doi.org/10.1021/acs.jcim.1c00918
25. Sk, M.F., Haridev, S., **Roy, R.** and Kar, P., **2021**. 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), pp.941-962. **DOI:** https://doi.org/10.1080/1062936X.2021.1999318
26. Sk, M.F., **Roy, R.**, Jonniya, N.A., Poddar, S. and Kar, P., **2021**. Elucidating 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), pp.3649-3661. **DOI:** https://doi.org/10.1080/07391102.2020.1768149
27. Sk, M.F., **Roy, R.** and Kar, P., **2021**. 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), pp.988-1003. **DOI:** https://doi.org/10.1080/07391102.2020.1724196
28. Thurakkal, L., Singh, S., **Roy, R.**, Kar, P., Sadhukhan, S. and Porel, M., **2021**. 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*, p.138193. **DOI:** https://doi.org/10.1016/j.cplett.2020.138193
29. Sk, M.F., Jonniya, N.A., **Roy, R.**, Poddar, S. and Kar, P., **2020**. 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*, p.590165. **DOI:** https://doi.org/10.3389/fmolb.2020.590165
30. **Roy, R.**, Ghosh, B. and Kar, P., **2020**. Investigating conformational dynamics of Lewis Y oligosaccharides and elucidating blood group dependency of cholera using molecular dynamics. ACS omega, 5(8), pp.3932-3942. **DOI:** https://doi.org/10.1021/acsomega.9b03398

Conference Publications:

1. Mukherjee A, Paul A, **Roy R**, Roy S, Ghosh K. Perceptual Filling-in of Blind-Spot for Surrounding Color Gradient Stimuli. ***International Conference on Intelligent Human Computer Interaction*** 2018 Dec 7 (pp. 194-204). Springer, Cham.

*Pre*sentations in *Con*ferences

1. Comprehensive Study of Structural Transitions between Protein Conformations *via* Adaptively Biased Path Optimization. ***39th Annual Symposium of The Protein Society***. (June 26-29, 2025). San Francisco, California. [**ORAL** & **POSTER**]
2. Exploring phosphorylation-driven interdomain dynamics between FAK's kinase and FERM domains through molecular dynamics. ***ACS Fall 2024***. (August 18-22, 2024). Denver, Colorado. [**ORAL**]
3. Consequences of Multisite Phosphorylation on the Structure of Focal Adhesion Kinase. ***SCBB/SBBC GRAD/POSTDOC Symposium***. (Dec 13, 2023). Purdue University. [**ORAL**]
4. Investigating Thermodynamics of Protein Structure with Multiscale Simulation and Machine Learning. ***Purdue Institute for Drug Discovery 8th Annual Symposium***. (Oct 6, 2023). Purdue University. [**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***. (May 16-17, 2023). Purdue University. [**POSTER**]

6. Effect of Sulfation on the Conformational Dynamics of Dermatan Sulfate Glycosaminoglycan: A Gaussian Accelerated Molecular Dynamics Study. ***44th Indian Biophysical Society Meeting***. (Mar 30-Apr 1, 2022). Advanced Centre for Treatment, Research and Education in Cancer, India. Online Conference. [**POSTER**]
7. Spatiotemporal Characterisations of Dermatan Sulphate Glycosaminoglycan Chains Through Enhanced Sampling. ***8th Annual Research Symposium at Centre for BioSystem Science and Engineering***. (Jan 28-29, 2022). Indian Institute of Science. Online Conference. [**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)*** (Sept 24-28, 2021). Online Conference. [**ORAL**]
9. Structural dynamics and recognitions of Lewis y oligosaccharides by cholera toxin: A molecular dynamics and free energy study. ***Computational Biology and Bioinformatics (CBB-2019)*** (July 31–Aug 1, 2019). Indian Institute of Technology Jodhpur. [**POSTER**]
10. Investigating Conformational Flexibility of *N*-Glycans via All-Atom Molecular Dynamics Simulations. ***International Conference on Mathematical Modelling and Scientific Computing (ICMMSC-2018)*** (July 19–21, 2018). Indian Institute of Technology Indore. [**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)*** (July 5–6, 2018). Indian Institute of Technology Indore. [**POSTER**]
12. Molecular Recognition of Drugs by Receptor Proteins via Multiscale Simulation Methods. ***5th Industry Academia Conclave (IAC)*** (Sept 6, 2017). Indian Institute of Technology Indore. [**POSTER**]

*Pro*ject Mentored

M.Sc. Dissertation

- ✓ Molecular Interaction Between Typhoid Toxin And *N*-linked Glycans: An *in-silico* Investigation | **Naveen Kumar** | *June, 2021- June, 2022* | at Indian Institute of Technology Indore
- ✓ Targeting SARS-CoV-2 spike protein with human metabolites: an in-silico study for drug development | **Rohit Kumar Singh** | *June, 2020 - June, 2021* | at Indian Institute of Technology Indore
- ✓ Drug binding analysis against a novel target in tuberculosis- a molecular dynamics approach | **Nima Tshering Bhutia** | *Dec, 2017 - Dec, 2018* | at Indian Institute of Technology Indore

Summer Trainee

- ✓ *In-silico* Investigation of Kinase Inhibitors against FMS like Tyrosine Kinase-3 | **Purushottam Behera** (NIT Rourkela); **Jyotirmoy Behera** (NIT Rourkela), **Yuvraj Rallapalli** (Manipal Institute) | *June-Aug 2021* | at Indian Institute of Technology Indore
- ✓ Understanding the recognition mechanism between Typhoid Toxin and Glycans | **Prarthita Rakshit** (NIT Durgapur), **Hari Om** (NIT Durgapur) | *June-Aug 2021* | at Indian Institute of Technology Indore

*Wor*kshops

Summer School On Machine Learning In Bioinformatics 2021 — *Online, Aug 23-27, 2021*
HSE University, Moscow, Russia

Simulation methods in scientific computing — *Online, June 14-16, 2021*
NSM NODAL CENTRE ON HPC & AI, INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR

Computational Approaches in Drug Design & Therapeutics — *Online, Feb 20, 2021*
DRUG DISCOVERY & DEVELOPMENT CLUSTER, AMITY INSTITUTE OF BIOTECHNOLOGY, AMITY UNIVERSITY CHHATTISGARH

Computational Biology and Bioinformatics — *Jodhpur, India, July 31-Aug 01, 2021*
INDIAN INSTITUTE OF TECHNOLOGY JODHPUR

Business Analytics using R — *Indore, India, March 20, 2019*
INDIAN INSTITUTE OF MANAGEMENT INDORE

Practical Protein Crystallography using PX Beamline at Indus-2 Synchrotron — *Indore, India, March 27-28, 2018*
RAJA RAMANNA CENTRE FOR ADVANCED TECHNOLOGY (RRCAT)

***In Silico* Analysis of Mutation** — *Indore, India, Dec 16, 2015*
UNIVERSITY OF KALYANI

*Pro*fessional Services

Reviewer in **Communications biology**
Reviewer in **Frontiers in Molecular Biosciences**
Reviewer in **Journal of Biomolecular Structure and Dynamics**
Reviewer in **Computers in Biology and Medicine**

*Ski*lls

Languages	**Bengali** (mother tongue), **English** (proficient), **Hindi** (conversational)
Programming	Python, R, FORTRAN, Shell Scripting, MATLAB, LATEX
Operating Systems	Linux, Windows
Scientific Software	CHARMM, AMBERGROMACS, NAMD, AutoDock, Schrödinger-Suite, UCSF Chimera, PyMOL, VMD

*Acc*omplishments

- **Grant Support** by Center for Indian Scientific Knowledge Systems (**CISKS**), IIT Indore
  - **Name:** In Silico Systematic Study of Ayurvedic Neuroprotective Herbs Against Dual Leucine Zipper Kinase for the Treatment of Neurodegeneration
  - **Role:** Principal Investigator
  - **Duration:** 9 months
- Qualified in **Graduate Aptitude Test in Engineering** 2017 with an *all-India Rank* of 153

*Cer*tifications

Building Transformer-based Natural Language Processing Applications — *Online, 2021*
NVIDIA DEEP LEARNING INSTITUTE

Fundamentals of Deep Learning — *Online 2021*
NVIDIA DEEP LEARNING INSTITUTE

Introduction to Computational Drug Design — *Online 2021*
SCHRÖDINGER & PHARMACY COUNCIL OF INDIA

Nano-biotechnology in Drug Discovery, Development and Delivery — *Indore, India 2021*
QIP, AICTE & INDIAN INSTITUTE OF TECHNOLOGY INDORE

Data Science and Analytics — *Indore, India 2020*
NPIU/TEQIP-III & INDIAN INSTITUTE OF TECHNOLOGY INDORE

GPU Computing in Computational Biology — *Indore, India 2020*
INDIAN INSTITUTE OF TECHNOLOGY INDORE

Introduction to Machine Learning — *Online June 2016*
NPTEL ONLINE CERTIFICATION & INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR

*Vol*unteer

Conferences:

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