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Post-Doctoral Research scholar
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Personal Details

Date of Birth: 4th October 1994
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West Bengal, India
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Educational Qualification

PhD in Life Sciences (09/10/2024)

Presidency University, Kolkata, India

Thesis title: "Studies on the conformational dynamics of HIV-1 accessory proteins to guide new therapeutic development"

M.Sc. in Life Sciences (09/11/2018) (CGPA: 9.35 out of 10), Presidency University, Kolkata, India

B.Sc. in Life Sciences (08/20/2016) (CGPA: 8.75 out of 10), Presidency University, Kolkata, India

Work Experience

Post-Doctoral Researcher (10/01/2024 – Present)

Department of Physics
University of Vermont
Burlington, VT 05405, USA

Project: "Molecular simulations and computer-aided drug discovery for treating cardiovascular diseases"

Awards and Honors

2021: Awarded Senior Research Fellowship, CSIR, Govt. of India
2018: Awarded Junior Research Fellowship, CSIR, Govt. of India
2017: Qualified UGC-CSIR(NET) exam for Junior research fellowship, All India Rank 72
Qualified UGC-CSIR(NET) exam for Junior research fellowship, All India Rank 114

Research profile

I have extensive experience in diverse computational techniques (classical Molecular Dynamics simulation, enhanced sampling methods, docking, etc.), and I leverage these skills to elucidate protein dynamics, accelerate drug discovery, and understand protein-ligand interactions. I am also highly proficient in advanced MD simulation methods like concentrated ligand docking (ColDock), supervised molecular dynamics (SuMD), and computational electrophysiology (CompEL) simulation. I also employ AI based molecular docking tools (e.g. GNINA, DiffDock) for large scale Virtual screening purposes. Complementing these efforts, I routinely develop Python codes to analyze and extract insights from MD simulation trajectories.

I have worked on the following projects:

- AI-Driven Large-Scale Virtual screening of small Molecules targeting β-Cardiac Myosin for the therapeutic management of Hypertrophic Cardiomyopathy (HCM).
- Investigation on the ion permeation process through Dengue virus M channel protein using a combination of Computational electrophysiology (CompEL) and SuMD simulations.
- Markov state modeling (MSM) of the conformational changes in the Dengue virus envelope protein.
- Modeling the possible Oligomeric form of the HIV-1 Vpr inside POPC lipid bilayer.
- Modeling the assembly process of the Dengue virus Membrane-Capsid-RNA complex.
- De novo generation of new drug like candidates and repurposing existing drugs to target viral proteins.
- Computer aided design of peptide based vaccine against Nipah virus and mammarenavirus.
- Computer aided design of nanobodies against Dengue virus Capsid protein.
- Mechanistic investigation of SpCas9 tolerance to PAM-distal mismatches using both experimental and computational approaches.

Computational skills

Molecular dynamics (MD) Simulation methods: Classical MD | Enhanced sampling methods (Metadynamics, Gaussian accelerated MD, Umbrella sampling, Steered MD) | Coarse-Grained (CG) MD simulation (MARTINI, CABS, UNRES) | multiple walker supervised MD (mwSuMD) simulation | Computational electrophysiology (CompEL) simulation | Concentrated ligand docking (ColDock) simulation | Random Acceleration Molecular Dynamics (RAMD)

Molecular dynamics Simulation packages: GROMACS | ACEMD | Desmond | AMBER

Visualization softwares: BIOVIA Discovery Studio | VMD | PyMol | Chimera

Molecular Docking programs: Any open-source program (Autodock | Autodock VINA | LeDock | AutoGrow4), AI-based docking program (GNINA, DiffDock, SurfDock)

Programming Language: Python

Language proficiency: English, Hindi, Bengali

List of Publications

2025

1. Chaudhuri D, **Majumder S**, Giri K. Computational Cross-Aggregation Study of Dengue Virus NS1, Capsid Anchor and 2k Peptides With Human Amylin, Aβ42 and α-Synuclein Peptides. *J Mol Recognit*. 2025 Sep;38(5):e70009. doi: 10.1002/jmr.70009. PMID: 40737183.

2. Chaudhuri D, Majumder S, Datta J, Giri K. Computational Insights on the Assembly of the Dengue Virus Membrane-Capsid-RNA Complex. J Membr Biol. 2025 Feb;258(1):75-96. doi: 10.1007/s00232-025-00337-4.

2024

3. Chaudhuri D, **Majumder S**, Datta J, Giri K. In silico fragment-based design and pharmacophore modelling of therapeutics against dengue virus envelope protein. *In Silico Pharmacol*. 2024 Sep 20;12(2):87. doi: 10.1007/s40203-024-00262-9. PMID: 39310675; PMCID: PMC11415559.

4. Chaudhuri D, Ghosh M, **Majumder S**, Giri K. Repurposing of FDA-approved drugs against oligomerization domain of dengue virus NS1 protein: a computational approach. *Mol Divers.* 2025 Apr;29(2):1619-1639. doi: 10.1007/s11030-024-10936-3. Epub 2024 Jul 17. PMID: 39017952.

5. Chaudhuri D, **Majumder S**, Datta J, Giri K. Repurposing of therapeutic antibodies against dengue virus envelope protein receptor binding domain. *Arch Microbiol*. 2024 Jun 20;206(7):312. doi: 10.1007/s00203-024-04039-8. PMID: 38900285.

6. Chaudhuri D, **Majumder S**, Datta J, Giri K. Computational Insights on the Assembly of the Dengue Virus Membrane-Capsid-RNA Complex. *J Membr Biol.* 2025 Feb;258(1):75-96. doi: 10.1007/s00232-025-00337-4.

7. Dey D, Chakravarti R, Bhattacharjee O, **Majumder S**, Chaudhuri D, Ahmed KT, Roy D, Bhattacharya B, Arya M, Gautam A, Singh R, Gupta R, Ravichandiran V, Chattopadhyay D, Ghosh A, Giri K, Roy S, Ghosh D. A mechanistic study on the tolerance of PAM distal end mismatch by SpCas9. *J Biol Chem.* 2024 Jun 3:107439. doi: 10.1016/j.jbc.2024.107439.

8. **Majumder S**, Deganutti G, Pipitò L, Chaudhuri D, Datta J, Giri K. Computational Insights into the Conformational Dynamics of HIV-1 Vpr in a Lipid Bilayer for Ion Channel Modeling. *J Chem Inf Model*. 2024 Apr 10. doi: 10.1021/acs.jcim.3c01859. Epub ahead of print. PMID: 38597744.

9. Chaudhuri D, Datta J, **Majumder S**, Giri K. Peptide based vaccine designing against endemic causing mammarenavirus using reverse vaccinology approach. *Arch Microbiol*. 2024 Apr 15;206(5):217. doi: 10.1007/s00203-024-03942-4. PMID: 38619666.

10. Chaudhuri D, **Majumder S**, Giri K. Repurposing of drugs targeting heparan sulphate binding site of dengue virus envelope protein: an in silico competitive binding study. *Mol Divers*. 2024 Apr 3. doi: 10.1007/s11030-024-10834-8. Epub ahead of print. PMID: 38570391.

11. Chaudhuri D, Ghosh M, **Majumder S**, Giri K (2024) Repurposing of FDA?approved drugs against oligomerization domain of dengue virus NS1 protein: a computational approach. *Mol Divers*. https://doi.org/10.1007/s11030-024-10936-3.

12. Chaudhuri, D., **Majumder, S.**, Datta, J., & Giri, K. (2024). Elucidating the conformational change of dengue envelope protein using the Markov state model. *Molecular Simulation*, 1–17. doi: 10.1080/08927022.2024.2387126

13. Chaudhuri D, **Majumder S**, Datta J, Giri K. Repurposing of therapeutic antibodies against dengue virus envelope protein receptor binding domain. *Arch Microbiol*. 2024 Jun 20;206(7):312. doi: 10.1007/s00203-024-04039-8. PMID: 38900285.

2023

14. Chaudhuri D, **Majumder S**, Datta J, Giri K. In silico designing of an epitope-based peptide vaccine cocktail against Nipah virus: an Indian population-based epidemiological study. *Arch Microbiol.* 2023 Nov 13;205(12):380. doi: 10.1007/s00203-023-03717-3. PMID: 37955744.

15. Maity J, **Majumder S**, Pal R, Saha B, Mukhopadhyay PK. Ascorbic acid modulates immune responses through Jumonji-C domain containing histone demethylases and Ten eleven translocation (TET) methylcytosine dioxygenase. *Bioessays.* 2023 Nov;45(11):e2300035. doi: 10.1002/bies.202300035. Epub 2023 Sep 11. PMID: 37694689.

16. Sarkar D, **Majumder S**, Giri K, Sabnam N. In silico characterization, molecular docking, and dynamic simulation of a novel fungal cell-death suppressing effector, MoRlpA as potential cathepsin B-like cysteine protease inhibitor during rice blast infection. *J Biomol Struct Dyn.* 2023 Oct-Nov;41(18):9039-9056. doi: 10.1080/07391102.2022.2139763. Epub 2022 Nov 8. PMID: 36345772.

17. Chaudhuri D, **Majumder S**, Datta J, Giri K. Exploring the chemical space for potential inhibitors against cell surface binding protein of Mpox virus using molecular fingerprint based screening approach. *J Biomol Struct Dyn.* 2023 Jul 22:1-14. doi: 10.1080/07391102.2023.2238087. Epub ahead of print. PMID: 37480263.

18. **Majumder S**, Deganutti G, Pipitò L, Chaudhuri D, Datta J, Giri K. Computer-aided de novo design and optimization of novel potential inhibitors of HIV-1 Nef protein. *Comput Biol Chem.* 2023 Jun;104:107871. doi: 10.1016/j.compbiolchem.2023.107871. Epub 2023 Apr 15. PMID: 37084691.

19. Chaudhuri D, Datta J, **Majumder S**, Giri K. Repurposing of drug molecules from FDA database against Hepatitis C virus E2 protein using ensemble docking approach. *Mol Divers.* 2023 Apr 16. doi: 10.1007/s11030-023-10646-2. Epub ahead of print. PMID: 37061608.

20. Datta J, **Majumder S**, Chaudhuri D, Giri K. In silico investigation of binding propensity of hematoxylin derivative and damnacanthal for their potential inhibitory effect on HIV-1 Vpr from different subtypes. *J Biomol Struct Dyn.* 2023;41(24):14977-14988. doi: 10.1080/07391102.2023.2184634. Epub 2023 Mar 1. PMID: 36858595.

2022

21. Chaudhuri D, Datta J, **Majumder S**, Giri K. In silico study on miRNA regulation and NSs protein interactome characterization of the SFTS virus. *J Mol Graph Model.* 2022 Dec;117:108291. doi: 10.1016/j.jmgm.2022.108291. Epub 2022 Aug 10. PMID: 35977432.

22. **Majumder S**, Chaudhuri D, Datta J, Giri K. Exploring the intrinsic dynamics of SARS-CoV-2, SARS-CoV and MERS-CoV spike glycoprotein through normal mode analysis using anisotropic network model. *J Mol Graph Model.* 2021 Jan;102:107778. doi: 10.1016/j.jmgm.2020.107778. Epub 2020 Oct 16. PMID: 33099199; PMCID: PMC7567490.

23. **Majumder S**, Giri K. An insight into the binding mechanism of Viprinin and its morpholine and piperidine derivatives with HIV-1 Vpr: molecular dynamics simulation, principal component analysis and binding free energy calculation study. *J Biomol Struct Dyn.* 2022;40(21):10918-10930. doi: 10.1080/07391102.2021.1954553. Epub 2021 Jul 23. PMID: 34296659.

24. Chaudhuri D, Datta J, **Majumder S**, Giri K. Prediction of infectivity of SARS-CoV-2 virus based on Spike-hACE-2 interaction. *Virusdisease.* 2022 Sep;33(3):244-250. doi: 10.1007/s13337-022-00781-z. Epub 2022 Aug 5. PMID: 35965884; PMCID: PMC9362045.

25. Chaudhuri D, **Majumder S**, Datta J, Giri K. Designing of nanobodies against Dengue virus Capsid: a computational affinity maturation approach. *J Biomol Struct Dyn.* 2023 Apr;41(6):2289-2299. doi: 10.1080/07391102.2022.2029773. Epub 2022 Jan 22. PMID: 35067204.

2021

26. Chaudhuri D, **Majumder S**, Datta J, Giri K. In Silico Study of Mutational Stability of SARS-CoV-2 Proteins. *Protein J.* 2021 Jun;40(3):328-340. doi: 10.1007/s10930-021-099883. Epub 2021 Apr 22. PMID: 33890205; PMCID: PMC8061876.

2020

27. Chaudhuri D, Datta J, **Majumder S**, Giri K. In silico designing of peptide based vaccine for Hepatitis viruses using reverse vaccinology approach. *Infect Genet Evol.* 2020 Oct;84:104388. doi: 10.1016/j.meegid.2020.104388. Epub 2020 May 30. PMID: 32485330.

Selected Presentations

- **Majumder S,** Giri K. "An insight into the effect of Viprinin and its Morpholine and Piperidine derivatives with HIV-1 Vpr: molecular dynamics simulation, principal component analysis and binding free energy calculation study". **Oral presentation** in the 4th Regional Science & Technology Congress (Southern Region), 2019, organized by Department of Science and Technology and Biotechnology, Government of West Bengal .

- **Majumder S,** Giri K. "Rational design of novel compounds through fragment based de novo approach against HIV-1 Nef to guide new antiretroviral therapy method". **Poster presentation** in the National conference on "Physiology to pathology: Finding the Therapeutic Roadmap" organized by Amity Institute of Biotechnology, Amity University, Kolkata during February 16-17, 2023.

- **Majumder S,** Giri K. "Designing novel drug like candidates against HIV-1 Nef using computational methods". **Poster presentation** in the two day International Conference (online) on "Biomolecules to Biome" held on August 24-25, 2022, organized by Department of Life Sciences, Presidency University, Kolkata, India.