
BIOGRAPHICAL SKETCH

Name: Pralay Mitra	Affiliation with contact details: Department of Computer Science and Engineering, Indian Institute of Technology Kharagpur, West Bengal – 721302, India Phone: +91-3222-282344 Email: pralay@cse.iitkgp.ac.in Home: http://cse.iitkgp.ac.in/~pralay/
Position Title: Professor	

A. Education/Training

Institution And Location	Degree	Duration	Field of Study
University of Michigan, Ann Arbor, USA	Postdoc	2011 – 2013	Computational Biology and Bioinformatics
Indian Institute of Science, Bangalore, INDIA	Postdoc	2010 – 2011	
Indian Institute of Science, Bangalore, INDIA	Ph.D.	2005 – 2010	
Bengal Engineering & Science University, Shibpur	M.E.	2002 – 2004	Computer Science & Engg
University of Calcutta, Kolkata, INDIA	B.Tech.	1999 – 2002	
University of Calcutta, Kolkata, INDIA	B.Sc. (H)	1996 – 1999	Physics, Math, Chemistry

B. Positions, and Employment

2025-present	Professor, Department of Computer Science and Engineering, IIT Kharagpur, India	
2020-2025	Associate Professor, Department of Computer Science and Engineering, IIT Kharagpur, India	
2013-2020	Assistant Professor, Department of Computer Science and Engineering, IIT Kharagpur, India	
2020-2025	Head, Institute Information Cell, IIT Kharagpur, India	
2020-2021	Associate Head, Centre for Computational and Data Sciences, IIT Kharagpur, India	
2015-2020	Associate Head, Institute Information Cell, IIT Kharagpur, India	
2012-2013	Senior Research Fellow, University of Michigan, Ann Arbor, USA	Supervisor: Prof. Yang Zhang
2011-2012	Research Fellow, University of Michigan, Ann Arbor, USA	
2010-2011	Research Associate, Indian Institute of Science, Bangalore, India	Supervisor: Prof. Debnath Pal
2006-2008	National Doctoral Fellow, All India Council for Technical Education, India	
2004-2005	Senior Computer Science Engineer, Avisere Technology Pvt. Ltd., India	

C. Honors, and Achievements

2018	Gandhian Young Technological Innovation Appreciation Award
2012	Our group scored an acceptable solution in CAPRI, Round 26, T-53
2011	My protein docking method scored acceptable solution in CAPRI, Round 24, T-50
2011	Award for Doctoral Thesis, Indian National Academy of Engineering
2005	Award for Master Thesis, Indian National Academy of Engineering
2004	University Silver Medal, Bengal Engineering and Science University, Shibpur
2004	Silver Medal in Computer Engineering, National Design, and Research Forum

D. Web servers and Software

Web servers developed and hosted at Indian Institute of Technology Kharagpur, India

DeepPROTECTNeo: Neo-antigen discovery for personalized cancer vaccines

rpcFold: Decipher RNA folding from RNA sequence

CAGETag: Predicts the Cap Analysis Gene Expression (CAGE) region from RNA sequences

ProTSPoM: Estimating Change in Protein Thermodynamic Stability owing to Single Point Mutation

PROFOUND: predicting PROtein FOldability owing to mUlti poiNt Deletions

Software developed

MaTPIP: Predicting Protein-Protein Interactions using Protein Language Model

PPSBoost: Predicting protein phosphorylation sites from protein sequence
ProDeMo: Parallel Protein Design Module
SPD_Pred: Encode the protein stability changes associated with single-point deletions (SPDs)
NIP_NSC: Calculate interface packing & surface complementarity at the biomolecular contacts

E. Peer-reviewed International Journal Publications

- ✓ Animesh, Suvvada, R., Bhowmick, PK., **Mitra, P.** (2025). E(Q)AGNN-PPIS: Attention Enhanced Equivariant Graph Neural Network for Protein-Protein Interaction Site Prediction *IEEE Transactions on Signal and Information Processing over Networks* 11:740-751
- ✓ Sarkar, S., Saha, S. A., Swarnakar, A., Chakrabarty, A., Dey, A., Sarkar, P., Banerjee, S., **Mitra, P.** (2024). The molecular prognostic score, a classifier for risk stratification of high-grade serous ovarian cancer. *Journal of Ovarian Research* 17(1):159 (14 pages)
- ✓ Nandi, S., Bhaduri, S., Das, D., Ghosh, P., Mandal, M., **Mitra, P.** (2024). Deciphering the Lexicon of Protein Targets: A review on Multifaceted Drug Discovery in the Era of Artificial Intelligence. *ACS Molecular Pharmaceutics* 21(4):1563–1590
- ✓ Ghosh, S., **Mitra, P.** (2024). MaTPIP: a deep-learning architecture with eXplainable AI for sequence-driven, feature mixed protein-protein interaction prediction. *Computer Methods and Programs in Biomedicine* 244:107955 (12 pages)
- ✓ Das, S., Kundu, M., Hassan, A., Parekh, A., Jena, B.C., Mundre, S., Banerjee, I., Yeitrajam, Y., Das, C.K., Pradhan, A.K., Das, S.K., Emdad, L., **Mitra, P.**, Fisher, P.B., Mandal, M. (2023). A novel computational predictive biological approach distinguishes Integrin β 1 as a salient biomarker for breast cancer chemoresistance. *Biochimica et Biophysica Acta - Molecular Basis of Disease (BBADIS)* 1869(6):166702 (17 pages)
- ✓ Sarkar, P., Banerjee, S., Saha, S.A., **Mitra, P.**, Sarkar, S. (2023). Genome surveillance of SARS-CoV-2 variants and their role in pathogenesis focusing on second wave of COVID-19 in India. *Scientific Reports* 13(1) Article number: 4692 (10 pages)
- ✓ Malik, A., Banerjee, A., Pal, A., **Mitra, P.** (2023). A sequence space search engine for computational protein design to modulate molecular functionality. *Journal of Biomolecular Structure & Dynamics* 41(7):2937-2946
- ✓ Biswas, A., Rajesh, A., Das, S., Banerjee, I., Kapoor, N., **Mitra, P.**, Mandal, M. (2022). Therapeutic targeting of RBPJ, an upstream regulator of ETV6 gene, abrogates ETV6-NTRK3 fusion gene transformations in glioblastoma. *Cancer Letters* 544:215811 (14 pages)
- ✓ Halder, P., **Mitra, P.** (2022). Human Prion Protein: Exploring the Thermodynamic Stability and Structural Dynamics of its Pathogenic Mutants. *Journal of Biomolecular Structure & Dynamics* 40(21):11274-11290
- ✓ Das, B., **Mitra, P.** (2022). ProMoCell and ProModb: web services for analyzing interaction-based functionally localized protein modules in a cell. *Journal of Molecular Modeling* 28(6):167 (8 pages)
- ✓ Pal, A., Mulumudy, R., **Mitra, P.** (2022). Modularity-based Parallel Protein Design Algorithm with an Implementation using Shared Memory Programming. *PROTEINS: Structure, Function, and Bioinformatics* 90(3):658-669
- ✓ Pal, B., **Mitra, P.** (2021). Protein Interaction Network-based Deep Learning Framework for Identifying Disease-Associated Human Proteins. *Journal of Molecular Biology* 433(19):167149 (15 pages)

- ✓ Pal, A., Pal, D., **Mitra, P.** (2021). A computational framework for modeling functional protein-protein interactions. *PROTEINS: Structure, Function, and Bioinformatics* 89(10):1353-1364
- ✓ Das, B., **Mitra, P.** (2021). High-performance Whole-cell Simulation Exploiting Modular Cell Biology Principles. *Journal of Chemical Information and Modeling* 61(3):1481-1492
- ✓ Banerjee, A., Pal, K. & **Mitra, P.** (2021). An evolutionary profile guided greedy parallel replica-exchange Monte Carlo search algorithm for rapid convergence in protein design. *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 18(2):489-499
- ✓ Banerjee, A., Kumar, A., Ghosh, K. K., **Mitra, P.** (2020). Estimating Change in Foldability due to Multi-point Deletions in Protein Structures. *Journal of Chemical Information and Modeling* 60(12):6679-6690
- ✓ Banerjee, A. & **Mitra, P.** (2020). Ebola Virus VP35 protein: modeling of the tetrameric structure and an analysis of its interaction with Human PKR. *Journal of Proteome Research* 19(11):4533-4542 (**The article is part of the Proteomics in Pandemic Disease special issue**)
- ✓ Biswas, A., Rajesh, Y., **Mitra, P.** & Mandal, M. (2020). ETV6 gene aberrations in non-haematological malignancies: A review highlighting ETV6 associated fusion genes in solid tumors. *Biochimica et Biophysica Acta - Reviews on Cancer* 1874(1):188389 (12 pages)
- ✓ Banerjee, A. & Mitra, P. (2020). Estimating the Effect of Single Point Mutations on Protein Thermodynamic Stability and Analyzing the Mutation Landscape of the p53 Protein. *Journal of Chemical Information and Modeling* 60(6):3315-3323
- ✓ Maiti, S., Hassan, A. & **Mitra, P.** (2020). Boosting phosphorylation site prediction with sequence feature-based Machine learning. *PROTEINS: Structure, Function, and Bioinformatics* 88(2):284-29
- ✓ Rajesh, Y., Banerjee, A., Pal, I., Biswas, A., Das, S., Dey, K.K., Kapoor, N., Ghosh, A.K., **Mitra, P.** & Mandal, M. (2019). Delineation of crosstalk between HSP27 and MMP-2/MMP-9: A synergistic therapeutic avenue for glioblastoma management. *Biochimica et Biophysica Acta - General Subjects* 1863(7):1196-1209
- ✓ Banerjee, A., Levy, Y. & **Mitra, P.** (2019) Analyzing change in protein stability associated with Single Point Deletions in a newly defined protein structure database. *Journal of Proteome Research* 18(3):1402-1410
- ✓ Shultis, D., **Mitra, P.**, Huang, X., Johnson, J., Khattak, N.A., Gray, F., Piper, C., Czajka, J., Hansen, L., Wan, B., Chinnaswamy, K., Liu, L., Wang, M., Pan, J., Stuckey, J., Cierpicki, T., Borchers, C.H., Wang, S., Lei, M. & Zhang, Y. (2019) Changing the Apoptosis Pathway through Evolutionary Protein Design. *Journal of Molecular Biology* 431(4):825-841
- ✓ Das, B., Patil, A.R., & **Mitra, P.** (2019) A Network-based Zoning for Parallel Whole-Cell Simulation. *Bioinformatics*. 35(1):88-94
- ✓ Maiti, S., & **Mitra, P.** (2018). Bacterial flagellar switching: a molecular mechanism directed by the logic of an electric motor. *Journal of Molecular Modeling*. 24:280
- ✓ Banerjee, A., Pal, A., Pal, D. & **Mitra, P.** (2018) Ebolavirus interferon antagonists—protein interaction perspectives to combat pathogenesis. *Briefings in Functional Genomics*. 17(6):392-401
- ✓ **Mitra, P.**, Shultis, D., Brender, J. R., Czajka, J., Marsh, D., Gray, F., Cierpicki, T. & Zhang, Y. (2013). An evolution-based approach to de novo protein design and case study on Mycobacterium Tuberculosis. *PLoS Computational Biology* 9(10): e1003298

- ✓ **Mitra, P.**, Shultis, D. & Zhang, Y. (2013). EvoDesign: de novo protein design based on structural and evolutionary profiles. *Nucleic Acids Research* 41: W273-W280. (**F1000Prime recommended**)
- ✓ Garma, L., Mukherjee, S., **Mitra, P.** & Zhang, Y. (2012). How many protein-protein interaction types exist in nature? *PLoS One* 7:e38913.
- ✓ **Mitra, P.** & Pal, D. (2011). PRUNE and PROBE – two modular web services for protein-protein docking. *Nucleic Acids Research* 39:W229-W234. (**Listed as OMIC-tools under Drug Discovery**)
- ✓ **Mitra, P.** & Pal, D. (2011). Combining Bayes classification and point group symmetry under Boolean framework for enhanced protein quaternary structure inference. *Structure* 19(3):304-312. (**Among Top 10 most read articles at Structure until April 2011**)
- ✓ **Mitra, P.** & Pal, D. (2011). Using correlated parameters for improved ranking of protein-protein docking decoys. *Journal of Computational Chemistry* 32(5):787-796.
- ✓ **Mitra, P.** & Pal, D. (2011). dockYard - a repository to assist modeling of protein-protein docking. *Journal of Molecular Modeling* 17(3):599-606.
- ✓ **Mitra, P.** & Pal, D. (2010). New measures for estimating surface complementarity and packing at protein-protein interfaces. *FEBS Letters* 584(6):1163-1168.
- ✓ **Mitra, P.**, Dhar, R. & Pal, D. (2009). Interface of apoptotic protein complexes has distinct properties. *In Silico Biol* 9(5-6):365-378.

F. Research Support

Project: 14 (running: 2; completed: 12)

Funded by: Indian Council of Medical Research, UGC under India-Israel Joint Research Project-2014; Indo-US Science and Technology Forum; SERB; National Supercomputing Mission; MHRD Department of Higher Education, New Delhi; IIT, Kharagpur

Collaborating Institutes:

International: University of California Los Angeles, USA; Weizmann Institute of Science, Israel; Los Alamos National Laboratory, USA; Virginia Commonwealth University, USA.

National: Indian Institute of Science Bangalore; Indian Institute of Technology Roorkee; Presidency University, Kolkata; All India Institute of Medical Sciences, Bhopal; Indian Institute of Chemical Biology, Kolkata

G. Research Students

	Degree	Students
Present	Ph.D.	12+2*
Completed	Ph.D.	4+1*
	National Post-doctoral Fellow	1
	Research Associate	1
	M.S. by research	1*
	M.Tech. & Dual Degree	43
	B.Tech.	22

*jointly supervised