Faculty CV

Name: Prof. Seema Mishra

Member, National Academy of Sciences, NASI, India

Editorial: npj Systems Biology and Applications

Designation: Professor

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Broad areas of research (only keywords)

Computational Oncology, Systems Biology, Molecular Biology, Computer-aided drug design, Immunoinformatics, Molecular dynamics

Professional Experience

Working as Professor in Department of Biochemistry, School of Life Sciences, University of Hyderabad, Hyderabad, India. Teaching and research in the area of Bioinformatics, Computational Biology and Systems biology.

Education/Training

Certificate course in Bioinformatics and Computational Biology from Supercomputing Facility for Bioinformatics and Computational Biology, Indian Institute of Technology-Delhi (IIT-D) and NIIT under the aegis of FITT in year 2004. First Division.

Ph.D. in Molecular Biology from National Institute of Immunology, Aruna Asaf Ali Marg, Near J.N.U., New Delhi. Awarded degree in year 2000. Thesis title: “Role of homologous region 1(hr1) in baculovirus AcNPV replication”. Supervisor: Padma Shri Prof. Seyed E. Hasnain.

M.Sc. in Biotechnology from Banaras Hindu University, Varanasi in year 1993. First Division. Special Paper: Plant Biotechnology. Paper title: “Regeneration studies in Cajanus cajan L.”

B.Sc. in Botany(Hons.) from Delhi University, Delhi in year 1991. First Division.

Senior Secondary School Certificate Examination in Science in year 1988. CBSE. First Division, Distinction in Biology, Physics, Maths and English.

Secondary School Certificate Examination in Science in year 1986. CBSE. First Division, Distinction in Science and English.

Detailed research interests (Upto 2 paragraphs or 10 bullet points)

Long non-coding RNAs in the regulation of gene expression in pan-cancer systems: We use these futuristic approaches in analyzing big data in cancers using a variety of tools ranging from machine learning (neural network) to interaction network studies to molecular dynamics. Specifically, our aim is to identify and establish interrelationships between coding (mRNA) and long non-coding (lncRNA) genes playing a key role in splicing, stability and degradation processes in pan-cancer development and progression. Their roles in pan-cancer drug resistance and sensitivity are also being analyzed to understand the molecular mechanisms. We aim to propose key regulatory paradigms of lncRNA molecules, such as *PVT1* and *MALAT1*. LncRNA structure-function studies in order to deduce function of known and unknown lncRNAs are also one of the many aims.

Artificial intelligence/machine learning tools in protein structure prediction: We use AlphaFold and RoseTTAFold in our work on studies on protein-protein interactions and protein-RNA complexes in health and disease. We also use machine learning methods such as ExtraTreeRegressor and Random Forest to study drug-protein target interactions and designing novel/repurposed drugs through machine learning-QSAR.

Computer-aided drug designing, Molecular dynamics to study drug-target interactions: We further use powerful molecular dynamics simulations to understand the structural basis of drug-protein target interactions in cancer occurring inside cells, and exploring the inside views of the consequential domain movements and essential conformational changes with atomistic accuracy.

Immunoinformatics in cancer immunotherapy: Applying immunoinformatics approaches to kickstart epitope-based vaccine development in cancers and SARS-CoV-2 has also been one of our frontrunner programs. The powerful approach of Immunoinformatics can be understood from the following observation: From thousands of potential epitopes generated computationally, and out of only two CTL epitopes of SARS-CoV-2 spike protein that were observed to be promiscuous (binding to several MHC class I supertypes) and immunogenic in big data Immunoinformatics studies conducted in March 2020 from my lab as a single author (Royal Society Open Science, September 2020), one CTL epitope (269-YLQPRTFLL-277) has been found generating the strongest CD8+ T cell responses in multiple independent studies using blood samples from convalescent patients (published in PNAS, 2020; Immunity, Nov and Dec 2020). This further reflects the timeliness of results and accuracy of computational tools well corroborated by independent experiments.

Selected publications (upto 5)

Selected Publications:

1. First publication from our Department from an M.Sc student as first author in a peer-reviewed International journal: Bhattacharjee R, Devi A and Mishra S* (2015). Molecular docking and molecular dynamics studies reveal structural basis and selectivity of inhibitors EGCG and OSU-03012 towards Glucose Regulated Protein-78 (GRP78) overexpressed in Glioblastoma. Journal of Molecular Modeling 21:272. * Ms. Rituparna has pursued her Ph.D in Germany. 2. Second-ever publication from our Department from an International M.Sc student from Sri Lanka as first author in a peer-reviewed International journal: Gurusinghe KRDSNS, Mishra A and Mishra S (2018) Glucose-regulated protein 78 substrate-binding domain alters its conformation upon EGCG inhibitor binding to nucleotide-binding domain: Molecular dynamics studies. Scientific Reports (Nature Publishing Group) 8:5487, DOI:10.1038/s41598-018-22905-6. *Mr. Sagara has pursued his Ph.D from Hebrew University of Jerusalem, Israel.

3. Saleembhasha A and Mishra S (2017) Novel molecules lncRNAs, tRFs and circRNAs deciphered from Next Generation Sequencing/RNA Sequencing: computational databases and tools. Briefings in Functional Genomics, 1-11, Oxford University Press. (doi: 10.1093/bfgp/elx013). 4. Saleembhasha A and Mishra S. (2019) Long non-coding RNAs as pan-cancer master gene regulators of associated protein-coding genes: a systems biology approach. PeerJ 7:e6388 https://doi.org/10.7717/peerj.6388

5. Mishra, S (2020) Designing of cytotoxic and helper T cell epitope map provides insights into the highly contagious nature of the pandemic novel coronavirus SARS-CoV-2, Royal Society Open Science, Royal Society Publishing 7:201141.

6. Roy Choudhuri KS and Mishra S (2020) Structural basis of BMP-2 and BMP-7 interactions with

antagonists Gremlin-1 and Noggin in Glioblastoma tumors, Journal of Computational Chemistry, 41:2544-2561, DOI: 10.1002/jcc.26407, Wiley (Publisher).

7. Kumar S and Mishra S (2022) MALAT1 as master regulator of biomarkers predictive of pan cancer multi-drug resistance in the context of recalcitrant NRAS signaling pathway identified using systems-oriented approach. Scientific Reports (Nature Publishing Group), DOI: 10.1038/s41598-022-11214-8

8. Mishra A, Mishra S (2024) MALAT1 lncRNA conformational dynamics in complex with RNPS1 in the pan-cancer splicing and gene expression. ACS Omega 9:42212-42226, https://doi.org/10.1021/acsomega.4c04467.

9. Sajal H and Mishra S (2025) An Innovative Machine Learning-Based QSAR approach for Prediction and Structural Analysis of Novel/Repurposed Acid Ceramidase (ASAH1) Inhibitors for Glioblastoma Therapy. Molecular Diversity (Springer Nature). https://doi.org/10.1007/s11030-025-11281-9

10. Kharsyiemiong ET, Raghunandan BH and Mishra S (2026) Structural basis of long non-coding RNA *PVT1* interactions with select mRNAs universal in pan-cancer systems: a computational study. Computational Biology and Chemistry (Elsevier).https://doi.org/10.1016/j.compbiolchem.2026.108878.

Selected projects (upto 5)

1. DBT Task Force on Bioinformatics, Project entitled ‘Systems biology and computational drug discovery for Mycobacterium tuberculosis active infection’. Sanctioned Rs 39,88,800.00. Sanction order BT/PR5535/BID/07/411/2012

2. UGC-SAP-DRS-1 grant to Department of Biochemistry, (with me as co-PI with other faculty of this Department) 1-4-2016 to 31-3-2021 (five years) Rs 108.50 lakhs (One crore, eight lakhs and fifty

thousands only) in two thrust areas: Interorganelle communication and dynamics, Simulation dynamics, Networks of signal transduction & Metabolic pathways INR 10850000.00 3. ICMR grant, "Integrative computational analysis of Omic data to explore novel intervention strategies towards breast cancer" co-PI, 2020.

4. DBT BIRAC Grant, "Designing, identification and validation of cytotoxic and helper T cell epitope based vaccine target candidates for novel coronavirus, SARS-CoV2 2019-nCoV" First round passed, did not qualify in second round.

5. DBT-Boost to University Interdisciplinary Life science Departments for Education and Research programme (BUILDER) Grant, Rs 50.44 crores to SLS, co- PI (2020).

6. UoH IoE grant entitled "Pan-cancer development: gene expression regulation by long non coding RNAs" sanctioned. Rs 5351140/- for 3 years (2021-2024).

Current PhD scholars and broad research topics

Ph.D and M.Sc Students

Ms. Euphinia Tiberius Kharsyiemiong

Mr. B H Raghunandan

Ms. Anamika Kumari

Dr. A. Saleembhasha Ph.D Working at NCI, NIH, Maryland, USA for Post-doc

Dr. Kesaban Ph.D Working at Medical College of Wisconsin, USA for Post-doc

Dr. Santosh Kumar Ph.D Working as Post-doctoral Visiting Fellow, NINDS, NIH, Maryland, USA

Ms. Soumi Mukherjee (M.Sc in our lab), working at Purdue University for Ph.D

Dr. Sagara N. S. Gurusinghe (M.Sc in our lab), worked at Hebrew University of Jerusalem, Israel, for his Ph.D.

Dr. Rituparna Bhattacharjee (M.Sc in our lab), worked at Ph.D from Otto-von-Guericke-University

Magdeburg

Dr. Amita Pal (M.Sc in our lab), Ph.D from UoH

Dr. S. Niranjan (M.Sc in our lab), Ph.D from UoH

Mr. Pankaj Kumar Chauhan (IM.Sc in our lab), PhD from NCBS

About 30 M.Sc students have done their dissertations from our lab, and continuing.