

IBS2025 Schedule

(Indian Institute of Technology Madras, March 6-9, 2025)

March 6, 2025 (Thursday) – ‘Cytiva Day’			
Time	Chair	Speaker	Venue
09:00 – 10:15		Registration, Coffee/Tea	TTJ Auditorium, IC & SR Building
10:15 – 10:30		Opening Remarks – Sudipta Maiti (President IBS, BITS Hyderabad)	
10:30 – 11:10	Ansuman Lahiri (Univ. of Calcutta)	Immunogen design to enhance stability and efficacy of viral vaccines Raghavan Varadarajan (IISc)	
11:15 – 11:55		Self-assembly of the Tau protein: Liquid-liquid phase separation and fibrillization Joan-Emma Shea (UC Santa Barbara, USA)	
12:00 – 12:20		Technical Talk - Cytiva	
12:20 – 14:00	Lunch (IC & SR Building Main Dining Hall, Dining Annex)		
14:00 – 14:40	P Karthe (Univ. of Madras)	β -Barrel chaperones: Multipoint assembly landscapes and lipid-regulated conformational plasticity Mahalakshmi R (IISER Bhopal)	TTJ Auditorium, IC & SR Building
14:45 – 15:25		Microbes and humans: A battle between membranes and pores Thomas Gutschmann (Research Center Borstel, Germany)	
15:30 – 15:50	Sudipta Maiti (BITS Hyderabad)	Meet the Editor: Prof. Joan-Emma Shea (ACS, JPC)	
15:50 – 16:30	Tea (IC & SR Building Main Dining Hall, Dining Annex)		
16:30 – 17:10	Hamsa Priya M (IIT Madras)	Molecular simulations as window into cellular dynamics Gerhard Hummer (Max Planck Inst. of Biophysics, Germany)	TTJ Auditorium, IC & SR Building
17:15 – 17:55		Modeling protein dynamics with machine learning and molecular simulation Cecilia Clementi (Freire Universität Berlin, Germany)	
18:00 – 18:15		Technical Talk – Zelle Biotech Twist Biosciences	
18:20 – 19:00		Molecular dynamics simulations and machine learning to investigate protein-ligand binding in [NiFe] hydrogenases Ariane Nunes Alves (Technical University Berlin, Germany)	
19:05 – 19:15		Technical Talk - Leica	
19:15 – 19:25		Technical Talk – Spinco Biotech	
19:25 – 19:35		Technical Talk – BD Biosciences	
19:40 – 21:00	Dinner (IC & SR Building Main Dining Hall, Dining Annex)		

IBS2025 Schedule

March 7, 2025 (Friday) – ‘Swayam Prabha Day’

Time Slot	Chair	Speaker	Venue		
09:00 – 10:00	Sudipta Maiti (BITS Hyderabad)	GN Ramachandran Lecture Biophysical journeys on fitness landscapes: from atoms to populations and back Eugene Shakhnovich (Harvard Univ., USA)	TTJ Auditorium, IC & SR Building		
10:00 – 10:20		Swayam Prabha (Prof. Arun Tangirala)			
10:25 – 10:45	Tea (IC & SR Building Main Dining Hall, Dining Annex)				
10:45 – 11:25	Sudipta Maiti (BITS Hyderabad)	Single-molecule FRET and FCS investigation of the interaction between SARS-CoV2 N protein and RNA Satoshi Takahashi (Tohoku University, Japan)	TTJ Auditorium, IC & SR Building		
11:25 – 12:05		Elucidating the mechanics and structure of whole mitotic chromosomes Gijs Wuite (Vrije Universiteit Amsterdam, Netherlands)			
12:10 – 12:20		Technical Talk – Jove			
12:20 – 12:30		Technical Talk – Toshniwal Bros.			
12:30 – 13:15		IBS General Body Meeting			
13:15 – 14:30	Lunch (IC & SR Building Main Dining Hall, Dining Annex)				
14:30 – 16:30	Poster Session 1 & Tea (Terrace Hall)				
Session 1 Microscopy and Single Molecules Venue TTJ Auditorium		Session 2 Biophysics Across Length Scales Venue Halls 1 & 3			
Time Slot	Sri Rama Koti Ainavarapu (TIFR Mumbai)	Speaker	Time	Anand Srivastava (IISc)	Speaker
16:30 – 16:50		<i>Changes in global RNA-protein metabolism during ageing cause alteration in stress granule properties</i> Shovamayee Maharana (IISc)	16:30 – 16:50		<i>Insights into the architecture and channel properties of Pannexins</i> Aravind Penmatsa (IISc)
16:50 – 17:10		<i>Structural and functional insights into Cren7: A DNA-bending protein from extremophiles</i> Soumit Mondal (IISER Tirupati)	16:50 – 17:10		<i>Role of metastable conformational states in proteins: From function to drug discovery</i> Suman Chakrabarty (SNBCBS)
17:10 – 17:30		<i>Insights into the malarial parasite cytoskeleton using cryo-electron microscopy</i> Mamata Banger (IIT Madras)	17:10 – 17:30		<i>Thermodynamics and kinetics of biomolecular recognition</i> Tarak Karmakar (IIT Delhi)
17:30 – 17:50		<i>Force-driven transformation of tunnel-associated chaperones: Unveiling a strain-energy-based mechanism for enhanced protein folding</i> Shubhasis Haldar (SNBCBS)	17:30 – 17:50		<i>Self-assembly pathway, energetics and morphology of peptide nanostructures</i> M Hamsa Priya (IITM)
17:50 – 18:10		<i>Replicating active transport of micro-organisms in synthetic systems</i> Sabyasachi Rakshit (IISER Mohali)	17:50 – 18:10		<i>F-actin architecture in the cytokinetic ring restricts E-cadherin mobility at furrow zone during cell division</i> Anup Padmanabhan (Ashoka Univ.)
18:10 – 18:30		<i>Sequence-dependent phase separation by Mycobacterium nucleoid-associated protein Lsr2 mediates DNA compaction</i> Mahipal Ganji (IISc)	18:10 – 18:30		<i>Physical confinement selectively favours bacterial growth based on cell shape</i> Tapomoy Bhattacharjee (NCBS)
18:30 – 18:50		<i>Determination of thermally induced cell membrane slope fluctuations using rotational optical tweezers</i> Basudev Roy (IITM)	18:30 – 18:50		<i>Polymer simulation study of the spatiotemporal organization of chromatin at the gene-length scale</i> Ranjith Pandinhateeri (IIT Bombay)
19:30 – 21:00	Dinner (Terrace Hall)				

IBS2025 Schedule

March 8, 2025 (Saturday)			
Time Slot	Chair	Speaker	Venue
09:00 – 09:40	Neelanjana Sengupta (IISER Kolkata)	Allosteric regulation of the restriction enzyme McrBC: towards deciphering the mechanism of activation of an endonuclease by a rotary motor Saikrishnan Kayrat (IISER Pune)	TTJ Auditorium, IC & SR Building
09:45 – 10:25		Decoding the rules of phase separation through minimalist peptide models and atomistic simulations David de Sancho (DIPC, Spain)	
10:25 - 10:50	Tea (IC & SR Building Main Dining Hall, Dining Annex)		
10:50 – 11:30	Neelanjana Sengupta (IISER Kolkata)	Physics of body axis formation Stephan Grill (MPI-CBG, Germany)	TTJ Auditorium, IC & SR Building
11:35 - 12:15		Combating ribosomal methylation based antibiotic resistance: A war at the microscopic level Ruchi Anand (IIT Bombay)	
12:20 – 12:30		Technical Talk – GeneX	
12:30 – 13:30	Lunch (Terrace Hall)		
13:30 - 15:30	Poster Session 2 & Tea (Terrace Hall)		
Session 3 Protein Structure and Mechanisms Venue TTJ Auditorium		Session 4 Computational Biophysics Venue Halls 1 & 3	
Time	Speaker	Time	Speaker
Preethi Raghunathan (Univ. of Madras)	<i>Ion channel-mediated regulation of excitatory/inhibitory (E/I) imbalance in Alzheimer's disease</i> Swagata Ghatak (NISER, Bhubaneswar)	15:30 – 15:50	<i>Uncovering high-resolution organization of genomic loci via multiscale polymer simulations</i> Arnab Bhattacharjee (JNU)
	<i>Fate of knotted proteins during directed degradation and constrained folding conditions</i> Hemachandra Kotamarthi (IITM)	15:50 – 16:10	<i>Exploring the energy landscapes of intrinsically disordered proteins using coarse-grained simulations</i> Debayan Chakraborty (IMSc)
	<i>A plausible mechanism of transcription activation of a subset of NF-kappaB repressed IRF3 target genes</i> Sulakshana Mukherjee (IISER Berhampur)	16:10 – 16:30	<i>Decoding thermosensation and associated response mechanisms in Caenorhabditis elegans</i> Rati Sharma (IISER Bhopal)
	<i>Profiling functional dynamics of high molecular weight proteins using solution NMR based methods at natural abundance</i> Subhabrata Majumder (SINP)	16:30 – 16:50	<i>Recent developments in integrative structural modeling of macromolecular assemblies</i> Shruthi Viswanath (NCBS)
	<i>Utilising simple building blocks for complex catalytic functions</i> Dibyendu Das (IISER Kolkata)	16:50 – 17:10	<i>Deciphering thermostability and structural dynamics in carbohydrate-active enzymes</i> Ragothaman Yenamalli (SASTRA)
	<i>Are the transmembrane domains of class I viral fusion proteins passive anchors or do they enable viral fusion?</i> Shachi Gosavi (NCBS)	17:10 – 17:30	<i>Dynamics of active tracer particles in complex environments: insights from computer simulations</i> Rajarshi Chakrabarti (IIT Bombay)
	<i>Glycans as attachment factor of SARS-CoV-2</i> Nagma Parveen (IIT Kanpur)	17:30 – 17:50	<i>Allosteric regulation of β-arrestin 1 and 2 effector specificity by GPCR phosphorylations</i> Rajesh Murarka (IISER Bhopal)
	Flash Talks – Session 1		18:00 – 19:00
Dinner (Terrace Hall)			

IBS2025 Schedule

March 9, 2025 (Sunday)			
Time Slot	Chair	Speaker	Venue
09:00 – 09:40	Sunil Kumar PB (IIT Madras)	A structure-based approach to tackle protein aggregation in Parkinson's disease Salvador Ventura (Autonomous Univ. of Barcelona, Spain)	TTJ Auditorium, IC & SR Building
09:45 – 10:25		Modeling DNA flexibility and its role in protein binding Martin Zacharias (Technical University Munich, Germany)	
10:30 – 10:40		Technical Talk - Nanotemper	
10:45 – 11:05	Tea (IC & SR Building Main Dining Hall, Dining Annex)		
11:05 – 11:45	Sunil Kumar PB (IIT Madras)	Unveiling the role of network stabilization in the aging dynamics of biomolecular condensates linked to neurodegenerative diseases Nunilo Cremades (University of Zaragoza, Spain)	TTJ Auditorium, IC & SR Building
11:50 – 12:30		Protein silencing with self-peptides Sudipta Maiti (BITS Hyderabad)	
12:35 – 13:15		Protein dynamics and kinetics studied by NMR spectroscopy Christian Griesinger (MPI- Göttingen, Germany)	
13:15 – 13:40	Student Awards, Closing Remarks (Dr. Hemachandra Kotamarthi , IIT Madras)		
13:00 – 15:00	Lunch (IC & SR Building Main Dining Hall, Dining Annex), Departure		

Flash Talks

Session 1 (TTJ Auditorium)			
Index	Name	Institute	Title of the Talk
1	Gaurav Kumar	University of York	Linker mediated phase separation of Rubisco in algal pyrenoids: a tale of stickers and spacers
2	Aravind R	NCBS	Plasticity of the proteasome-targeting signal Fat10 enhances substrate degradation
3	Aruldoss Immanuel	SASTRA Deemed to be University	Computational modelling of Levan Biosynthesis pathway in <i>Bacillus subtilis</i> : Implications in strain optimization and engineering
4	Parthasarathi Sahu	National Institute of Technology Durgapur	Efficient replication and information storage capacity sets the genome length
5	Ankush Garg	Aarhus University	Oxygen partitioning into biomolecular condensates is governed by protein density
6	Arya Krishna	Rajiv Gandhi Centre for Biotechnology	Conformational Dynamics of Membrane Porins Control Cyclic Sugar Transport
7	Chandrasekaran Prabaharan	International Institute of Molecular and Cell Biology	Structural and biochemical characterization of cauliflower mosaic virus reverse transcriptase
8	Priyotosh Sil	The Institute of Mathematical Sciences (IMSc), Chennai	Biologically meaningful regulatory logic enhances the convergence rate in Boolean networks and bushiness of their state transition graph
9	Takahiro Kimura	Tohoku University	Single-molecule FRET investigation on the long-range contact formation in the folding of a gRNA granule of SARS-CoV-2
10	Aditya Shrivastava	Tata institute of fundamental research	Ionic Liquid-Induced Modulation of Ubiquitin Stability: The Dominant Role of Hydrophobic Interactions
Session 2 (Hall 1 & Hall 3)			
Index	Name	Institute	Title of the Talk
1	Suman Pal	IISER Pune	Phase Transitions of mammalian Prion Protein: Molecular Mechanisms, Structural Insights, and Disease Relevance
2	Harini SureshKumar	Indian Institute of Science	Emergence of soft dynamic channels in highly ordered lipid bilayers
3	Anjana Peethambaran Menon	Indian Institute of Technology Bombay	Decoding the role of mycobacterial lipid remodelling and membrane dynamics in antibiotic tolerance
4	Mahima	Indian Institute of Technology Jammu	The Dual Influence of Transcriptional and Translational Kinetics on Gene Expression Noise
5	Aarcha Radhakrishnan	Institute of Nanoscience and Technology, Punjab	Bio-nanoreactor formation using BMC shell protein by probing the role of disordered regions of enzyme cargoes
6	Anjana V M	National Institute of Technology Karnataka	What drives vesicle formation in peptide permeation through the cancerous membrane: Insights from umbrella sampling simulations

7	Saloni Goyal	Indian Institute of Technology Madras	Polyphosphate Discriminates Protein Conformational Ensembles More Efficiently than DNA Promoting Diverse Assembly and Maturation Behaviors
8	Smriti Mukherjee	CSIR-Central Leather Research Institute (CSIR-CLRI)	Engineering Collagen Mimicry with Short, Hyperstable Collagen-Mimetic Peptides via Terminal π -Capping
9	Sukanya Sadhu	Raman Research Institute	Bi-Directional DNA Translocation in Conical Nanopores

Poster Presentation Schedule

March 7, 2025 (14:30 – 16:30) (Terrace Hall)

Session 1

Index /Poster No.	Name	Institute	Title of the Poster
1	Abdul Basit	Jawaharlal Nehru University	Reliability of Calcium-Binding Site Prediction with AlphaFold 3: Insights from Analysis of Crystal Structure
2	Aditi G Muddebihalkar	Indian Institute of Technology Madras	Unlocking the Puzzles of Self-Assembly and Disassembly of Viral Capsid
3	Aishani Tewari, Gayatri Tendulkar	Krea University	Benchmarking Computational Models for Relaxation Dispersion NMR: Insights into Sub-Millisecond Protein Dynamics
4	Anjana V Mathath	National Institute of Technology Surathkal	What drives vesicle formation in peptide permeation through the cancerous membrane: Insights from umbrella sampling simulations
5	Anusree Sen	S. N. Bose National Centre for Basic Sciences	Alteration at a Protein-Water interface due to changes in pH
6	Aravind R	National Center for Biological Sciences, Tata Institute of Fundamental Research (NCBS), India	Plasticity of the proteasome-targeting signal Fat10 enhances substrate degradation
7	Aruldoss Immanuel	SASTRA Deemed to be University	Computational modelling of Levam Biosynthesis pathway in <i>Bacillus subtilis</i> : Implications in strain optimization and engineering
8	Bhanu Priya	Indian Institute of Technology Madras	Investigating The Influence of Solvent on Self-Assembly Mechanism of Peptides
9	Bharath Raj P	Indian Institute of Technology Madras	Molecular Insights into CETP-Mediated Lipid Transfer and Inhibition Mechanisms
10	Bhavna Chaudhary	Indian Institute of Technology Madras	Influence of Cardiolipin on Bacterial Membrane Dynamics Under Osmotic Stress
11	Dhruv Kumar Chaurasiya	Indian Institute of Technology Madras	The thermodynamic architecture of eukaryotic protein kinase
12	Digvijay Lalwani Prakash	National Center for Biological Sciences, Tata Institute of Fundamental Research (NCBS), India	SuBMIT: A Toolkit for Facilitating Simulations of Coarse-Grained Structure-Based Models of Biomolecules.
13	Gugan Kothandan	University of Madras	Predictive modeling to forecast SARS-COV-2 variants and understanding its virulence by integrating machine learning and biophysical studies
14	Harini SureshKumar	Indian Institute of Science, Bengaluru	Emergence of soft dynamic channels in highly ordered lipid bilayers
15	Jaya Vasavi Pamidmukkala	Indian Institute of Technology Madras	An integrative computational approach to predict viral epitopes by targeting the MHC-TCR complexation
16	Kartik Majila	National Center for Biological Sciences, Tata Institute of Fundamental Research (NCBS), India	A deep learning method for predicting interactions for intrinsically disordered proteins

17	Kavana Priyadarshini Keshava	Jawaharlal Nehru University	From Contacts to Patterns: Quantifying Structural Changes in HIC data
18	Kompella V K Srinath	Aganitha.ai, Jubilee Hills, Hyderabad	Synergizing Physics-based modeling with AI/ML for BioPharma R&D
19	Koushik Ghosh	National Institute of Technology Durgapur	Non-enzymatic Kinetic Error Correction in Primordial Nucleotide Replication through Asymmetric Cooperativity
20	Madhurima Khamaru	Presidency University	An insight into the leucine zippers present in the unique blue light photoreceptor of marine alga <i>Ectocarpus siliculosus</i>
21	Mahima	Indian Institute of technology Jammu	The Dual Influence of Transcriptional and Translational Kinetics on Gene Expression Noise
22	Menaka Thambiraja	SASTRA Deemed to be University	Computation Analysis of Pathogenic Variants in the POLG2 and TWNK Mitochondrial Proteins.
23	Nisha Nandhini Shankar	SASTRA Deemed to be University	Family-level characterization of lytic polysaccharide monoxygenases using multiscale modeling
24	Parthasarathi Sah	National Institute of Technology Durgapur	Efficient replication and information storage capacity sets the genome length
25	A Dhanusha	Bharathidasan University	Graphene Hybrid Scaffolds for Laser Stimulated Neuro-regeneration
26	Aarcha Radhakrishnan	Institute of Nanoscience and Technology, Punjab	Bio-nanoreactor formation using BMC shell protein by probing the role of disordered regions of enzyme cargoes
27	Aditya Shrivastava	Tata Institute of Fundamental Research, Mumbai	Ionic Liquid-Induced Modulation of Ubiquitin Stability: The Dominant Role of Hydrophobic Interactions
28	Ahana Banerjee	CSIR-Indian Institute of Chemical Biology, Kolkata	Exploring Liquid-Liquid Phase Separation in ALS-Associated SOD1 Mutants
29	Aishi Dasgupta	IITB-Monash Research Academy	Characterization of SARS-CoV-2 Pseudoviruses: Investigating Spike Protein Interactions with Mammalian Cells at Membrane and Global Levels
30	Ajit Seth	Shiv Nadar Institution of Eminence	Hydrophobicity Dependent Deformation of Bacterial Cell Wall Induced by Imidazolium-Based Ionic Liquids
31	Akhil K Mohan	CSIR-National Institute for Interdisciplinary Science and Technology (NIIST), Trivandrum	Outer Membrane Vesicle-Derived Membrane Model for Probing the Peptide Interactions
32	Anagha C Unnikrishnan	CSIR-Central Leather Research Institute (CSIR-CLRI)	Dominance of Hydrogen Bonding over Aromatic π - π Interactions in the Efficiency of Peptide Gelators in Supramolecular Hydrogelation: Asparagine as a Key Factor
33	Anirban Mullick	National Institute of Technology Tiruchirapalli	Confirmatory detection and evaluation of acid rain stress in Neem (<i>Azadirachta indica</i>) using spectroscopic techniques
34	Anjali D. Patil	CSIR-National Chemical Laboratory	Functional Nucleic-Acid Binding Domain Of TAR-DNA Binding Protein-43 Forms Pathogenic Beta-Aggregates Via Monomeric Early Precursor Intermediate
35	Anjana P Menon	Indian Institute of Technology Bombay	Decoding the role of mycobacterial lipid remodelling and membrane dynamics in antibiotic tolerance
36	Ankush Garg	Aarhus University	Oxygen partitioning into biomolecular condensates is governed by protein density
37	Ankush Roy	Indian Institute of Science, Bengaluru	Structural Analysis of Broadly Neutralizing Antibody Interactions with Dengue Virus.
38	Aravinth S	Indian Institute of Science, Bengaluru	Measuring Chirality of Single Protein Molecule in a Cellular Environment Using Localization Microscopy
39	Arkabrata Mishra	Raman Research Institute	Understanding of mechanical heterogeneity in cells by resistive pulse sensing using glass microchannel
40	Arnab Bhattacharya	Saha Institute of Nuclear Physics	Probing the structural changes in therapeutic IgG1 mAbs by solution NMR based fingerprinting at natural abundance

41	Arnab Ghosh	Indian Institute of Science, Bengaluru	Structural and pharmacological insights into Noradrenaline reuptake inhibition
42	Arya Krishna	Rajiv Gandhi Centre for Biotechnology, Thiruvananthapuram	Conformational Dynamics of Membrane Porins Control Cyclic Sugar Transport
43	Avinash Chettri	University of Potsdam	2D-IR Spectroscopy Shows the Influence of Sequence Specificity on the Macrostructure of Single-Repeat GLFG Hydrogels.
44	Aysha Fahmeetha	National Center for Biological Sciences, Tata Institute of Fundamental Research (NCBS), India	Translational regulation by Huntingtin and its Rhes-mediated pathogenesis in Huntington's Disease
45	Ayushi Srivastava	Indian Institute of Science, Bengaluru	Investigation into a multi-domain transporter reveals new modes of allosteric regulation in cation: H ⁺ antiporters
46	Bhavika Gupta	Indian Institute of Technology Bhubaneswar	The N-Terminal domain of Mycobacterium leprae HSP18: Key to its structural integrity and chaperone activity
47	Chandrasekaran Prabaharan	International Institute of Molecular and Cell Biology in Warsaw	Structural and biochemical characterization of cauliflower mosaic virus reverse transcriptase
48	Debodyuti Sadhukhan	BRIC National Institute of Immunology	Structure-function relationship studies of a mitochondrial protein MRPL50
49	Devasena Umair R	Indian Institute of Technology Madras	pH and chemical induced denaturation of Esterase from Clostridium acetobutylicum
50	Dimple Goel	Institute of Nanoscience and Technology, Punjab	Engineering Bacterial Microcompartments: Insights from Shell Protein Interaction Studies
51	Dipam Naskar	Homi Bhabha National Institute, Mumbai & NISER Bhubaneswar	Dissecting the pathophysiology of full-length human Tau as an IDP and the spread function of neuro-degeneracy through protein-membrane interaction
52	Gaurav Kumar	University of York	Linker mediated phase separation of Rubisco in algal pyrenoids: a tale of stickers and spacers
53	Harshita Dutta	Indian Institute of Science, Bengaluru	Role of RNA pseudoknot antitoxin in type III toxin-antitoxin complex assembly and toxin inhibition
54	Indu	Jawaharlal Nehru University	Understanding the mechanism of human gamma D-crystallin aggregation at acidic and physiological pH
55	Irawati Roy	Indian Institute of Science, Bengaluru	Unambiguous assignment of kinked beta sheets leads to insights into molecular grammar of reversibility in biomolecular condensates
56	Jayashree Ravi	University of Madras	Systematic Biophysical Approach to Study Plastic Degradation: Polycaprolactone (PCL) Degradation by Mycobacterium marinum Cutinase
57	Jayita Biswas	Indian Association for the Cultivation of Science, Jadavpur	Molecular crosstalk between ectodomains of adherens junction proteins, E-cadherin and Nectin-4
58	Judith Gracia	University of Madras	Investigation of Amlodipine Besylate and Ranitidine Hydrochloride as Bacterial RNA Polymerase inhibitors
59	Kalpaja Acharya	National Center for Biological Sciences, Tata Institute of Fundamental Research (NCBS), India	A study of aggregation kinetics of Poly-ubiquitin fibrils
60	Koushik Chalki	Tata Institute of Fundamental Research, Mumbai	Investigating the Mechanical Response of Parallelly Arranged Polyproteins: Mimicking the Mechanical Stress in Biological Systems
61	Koustav Saha	Indian Institute of Technology Guwahati	Bridging the Knowledge Gap: Investigating K18 and K19 aggregation through Protein Charge Transfer Spectra (ProCharTS)
62	Arkadeep Banerjee	NCBS-TIFR, Bengaluru	Understanding Self-Peptide Insertion During Protein Folding

63	M Abith	Bharathidasan University	Silver Incorporated Reduced Graphene Oxide-Molybdenum Disulfide (Ag-rGO-MoS ₂) Hybrid Material for Bio-phonic Application
64	Mahesh Yadav	Institute of Physics, Johannes Gutenberg University	Phase transitions in intrinsically disordered RNA binding proteins and crucial role of RGG motifs
65	Mani Gupta	Jawaharlal Nehru University	Exploring the anti-fibrillating effect of the anthocyanidin Petunidin on the aggregation and amyloid fibril formation of α -synuclein involved in Parkinson's disease
66	Megha Rai	Ashoka University	ARP-2/3 regulates cell surface dynamics of CeTOCA-1 in the <i>C. elegans</i> zygote
67	Mona S. Kirmire	CSIR-National Chemical Laboratory	Phase Separation Dynamics of FLTP-43: A Protective Mechanism or Pathological Driver in Neurodegeneration?
68	Muskaan Jindal	National Center for Biological Sciences, Tata Institute of Fundamental Research (NCBS), India	Integrative structure determination of sub-complexes of the mitochondrial contact site and cristae organizing system (MICOS)
69	Nafisa Siddiqui	Indian Institute of Science Education and Research (IISER) Bhopal	A first passage time study of bacterial eradication under the influence of antibacterial agents

March 8, 2025 (13:30 – 15:30) (Terrace Hall)

Session 2

Index /Poster No.	Name	Institute	Title of the Poster
1	Prashanta Swain	Indian Institute of Technology Madras	Unravelling the Influence of Cholesterol and Membrane Composition on Drug Transport Dynamics
2	Prithviraj Uttarasili	Indian Institute of Science, Bengaluru	Extent of stochasticity in folding dynamics determines the force-tolerance and longevity of mechanosensing proteins
3	Priyanka Yadav	Indian Institute of Technology Hyderabad	Mechanistic of repeat RNA folding and its interaction with drug molecule using molecular dynamics simulations
4	Priyotosh Sil	The Institute of Mathematical Sciences (IMSc), Chennai	Biologically meaningful regulatory logic enhances the convergence rate in Boolean networks and bushiness of their state transition graph
5	Raghav Mathur	Indian Institute of Science, Bengaluru	Effect of Hydropathy Scale on Intrinsically Disordered Protein Properties Predicted using Implicit Solvent Simulations
6	Rupal Chauhan	Indian Institute of technology Jammu	Non-Equilibrium Kinetics of Chaperone Molecules in Protein Folding
7	Saanya Yadav	Indian Institute of Technology Hyderabad	Structure and self-assembly of DNA nanostructure in lipid bilayer membrane
8	Sahil Lall	National Center for Biological Sciences, Tata Institute of Fundamental Research (NCBS), India	A hydrophobic mismatch in the transmembrane helices of class I viral fusion proteins may facilitate viral fusion
9	Santosh Prajapati	Indian Institute of Science, Bengaluru	π - π and cation- π interactions are required in intrinsically disordered protein coarse-grained models to recapitulate experimental reality
10	Sashikanta Barik	National Institute of Technology Durgapur	Evolutionary and Functional Insights Among CRISPR-Cas Systems Through Direct Repeat Analysis
11	Satya Chaithanya Duggisetty	Indian Institute of Science, Bengaluru	NBAR-mediated membrane deformations at multiples scales using integrated continuum mechanics and molecular simulations
12	Shilpi Singh	Indian Institute of Technolog Delhi	Understanding RNA Chaperon Activity of ProQ Protein using Molecular Dynamics and Enhanced Sampling Method

13	Shourya Burnwal	IISER Pune	Beyond annotation: Identifying potential proteins in <i>D. melanogaster</i> and <i>C. elegans</i>
14	Sk Habibullah	Indian Institute of Science, Bengaluru	Metal Ion Driven Folding of GAAA Tetraloop Receptor Complexes
15	Smita Manjari Panda	Indian Institute of Technology (Indian School of Mines), Dhanbad	Unveiling a Novel Inhibitor of EGFR Tyrosine Kinase: An In-Silico study
16	Soham Choudhuri	International Institute of Information Technology, Hyderabad	Computational approach for decoding malaria drug targets from single-cell transcriptomics and finding potential drug molecule
17	Sumitro Dey	Indian Institute of Technology Hyderabad	Structure, dynamics small molecule modified DNA Hydrogel
18	Sunita Muduli	Indian Institute of Science, Bengaluru	Dynamics of Broadly Neutralizing Antibody Interactions and Glycan Modulation in Glycosylated HIV-1 Env: A Clade-Specific Perspective from Molecular Dynamics Simulations and Machine Learning Approaches
19	Sweetie Deena Ramesh	SASTRA Deemed to be University	Mathematical modelling of cellulose and chitin degradation in the presence and absence of lytic polysaccharide monoxygenases
20	Truptimayee Das	International Institute of Information Technology (IIIT) Bhubaneswar	A Comparative Study of Electrical Activity in Human Cardiac Cell Models: The Effects of Pacing and Ionic Conductance on EADs
21	Vijay Subramanian	IISER Pune	Morpheus: An Fragment-based Algorithm to Predict Metamorphic Behaviour in Proteins
22	Vinodhini Selvanarayanan	Indian Institute of Science, Bengaluru	Molecular design principles underlying the conformational dynamics diversity in EHD paralogs
23	Yogendra Kumar	Indian Institute of Science, Bengaluru	siRNA complexation with Galactose-Functionalized Dendrimer: PAMAM vs PETIM
24	Pankaj Adhikary	Indian Institute of Technology Tirupati	Validation of various urea force fields through vibrational spectroscopy and interface surface area
25	Piu Sarkar	Presidency University	Characterization of Aureochromes: A unique Photoreceptor cum Transcription Factor
26	Preeti Negi	Institute of Nanoscience and Technology, Punjab	Exploring the Interplay Between Bacterial Microcompartments and Outer Membrane Vesicles in Salmonella Pathogenesis
27	Pritam Saha	Indian Institute of Science Education and Research Mohali	Extent of stochasticity in folding dynamics determines the force-tolerance and longevity of mechanosensing proteins
28	Punitkumar Nagpure	Raman Research Institute	Detection and Characterization of DNA-Cas9 Interactions Using Glass Nanopores
29	Pushpakant Sahu	Indian Institute of Technology Madras	Probing the oligomerization/de-oligomerization process of Mtb's ATPase, Mpa
30	Lawanya Natarajan	Indian Institute of Technology Madras	Sequestration Mechanisms in MerR Family Antibiotic Binding Proteins
31	Rasanpreet Kaur	Indian Institute of Technology Guwahati	Decoding the Structural insights of Prothymosin- α by novel label-free approach: Protein Charge Transfer Spectra
32	Rishav Barman	Indian Institute of Science, Bengaluru	A MarR/DUF24 family transcriptional regulator directs bacterial nanotube formation
33	Ritu Raj	Indian Institute of Technology Madras	Impact of Nucleosome Dynamics on Condensed Chromatin Globules
34	Sakshi Priyadarsini Dutta	Indian Institute of Technology Bhubaneswar	Impact of Multidrug Therapy Drugs on the Structure and Chaperone Function of Mycobacterium tuberculosis Hsp16.3
35	Saloni Goyal	Indian Institute of Technology Madras	Polyphosphate Discriminates Protein Conformational Ensembles More Efficiently than DNA Promoting Diverse Assembly and Maturation Behaviors
36	Sandeep Ameta	Ashoka University	Constraints of liquid-liquid phase separated droplets

37	Sangeetha Balasubramanian	Indian Institute of Science, Bengaluru	Unravelling the origin of polymorphic behavior in G-quadruplexes using integrated NMR spectroscopy and all-atom molecular dynamics simulations
38	Sankha Shuvra Das	Raman Research Institute Bangalore	A Futuristic Microfluidic Platform for SiHa Cancer Cell Sorting and Stiffness Profiling
39	Saswati Soumya Mohapatra	Indian Institute of Technology, Bhubaneshwar	Unravelling anti-amyloidogenic and fibril-disrupting effects of a gut microbiota metabolite on insulin fibrillation through multispectroscopic, machine learning and hybrid QM/MM approaches
40	Satyendra Rajput	Indian Institute of Technology Delhi	Role of Attractive Crowder Interactions in the Hydration Shell Driving Biomolecular Aggregation, Collapse, and Folding
41	Saamyadeep Goswami	Indian Institute of Technology Kharagpur	Elucidating the structural and functional aspects of the novel heterophilic interaction between E-cadherin and nectin-4
42	Sazida	BRIC National Institute of Immunology	Elucidating the Molecular Mechanism of Thioesterase 2-Acyl Carrier Protein Interaction
43	Shakya Sinha	Saha Institute of Nuclear Physics	Probing the mechanistic basis of the redox regulated chaperon Hsp33 activity
44	Shilpi Laha	Indian Institute of Technology Madras	Phosphorylation Acts as a Switch Inducing Destabilization and Controlling Context-Dependent Phase-Separation in HMG Proteins
45	Shivangi Vaish	BRIC National Institute of Immunology	Structural characterization of mitochondrial acyl carrier
46	Shyla Singh	Vrije Universiteit Amsterdam	BLM helicase unwinding mechanisms: Implications for DNA repair and genome maintenance
47	Yogita	BRIC National Institute of Immunology	Characterization of Fatty Acid Synthase (FasN): a multimeric enzyme complex
48	Smriti Mukherjee	CSIR-Central Leather Research Institute (CSIR-CLRI)	qEngineering Collagen Mimicry with Short, Hyperstable Collagen-Mimetic Peptides via Terminal π -Capping
49	Snehasis Sarkar	Indian Institute of Science Education and Research Mohali	Chaperone-Mediated Phase Separation Modulates the Liquid-to-Solid Transition of an Amber Stop Codon Mutant of the Prion Protein (Y145X)
50	Soham Mukherjee	Indian Institute of Technology Madras	Mechanical degradation and unfolding studies of knotted proteins using single molecule force spectroscopy
51	Sombuddha Sengupta	Indian Institute of Technology Bombay	Structural and Functional Basis of Erm-Mediated Antibiotic Resistance
52	Spandan Basu	Indian Institute of Science, Bengaluru	Establishing the organization of cellular condensates in aging
53	Sreelakshmi Radhakrishnan	CSIR- National Institute for Interdisciplinary Science and Technology (NIIST), Trivandrum	Dynamic Coacervate-lipid membrane Interaction Regulates Membrane Bending
54	Srividhya S	Indian Institute of Science, Bengaluru	Immune Recognition of Dengue Virus: A Structural Analysis of Surface Epitopes
55	Subbulakshmi Sakthivel	University of Madras	Structural and functional studies of the enzyme PseF involved in pseudaminic acid biosynthesis pathway from Helicobacter pylori
56	Subhrodeep Saha	Indian Institute of Science, Bengaluru	Miniprotein-Driven IgG Oligomerization for Targeting Protein-Protein Interactions
57	Subir Chatterjee	Indian Institute of Science, Bengaluru	Understanding the design of ultrastable α - helical hairpin motif
58	Neptune Baro	Indian Institute of Science, Bengaluru	Two-Dimensional Light-Sheet Optical Tweezer (2D-LOT) Facilitates the Trapping and Imaging of Live Cells in a Selective Plane
59	Sudipta Mondal	University of Pittsburgh	Interaction dynamics of mycobacteria and phage revealed by in-situ cryo-electron tomography

60	Suganthi C	Sri Sivasubramaniya Nadar College of Engineering, Kalavakkam	Exploring the interaction between Protein Z dependent Protease Inhibitor (ZPI) and Plasma Pre-kallikrein
61	Sukanya Sadhu	Raman Research Institute	Bi-Directional DNA Translocation in Conical Nanopores
62	Suman Pal	Indian Institute of Science Education and Research Pune	Phase Transitions of mammalian Prion Protein: Molecular Mechanisms, Structural Insights, and Disease Relevance
63	Suman Tiwary	Tata Institute of Fundamental Research, Mumbai	Electrostatics dominate Au-S interaction in governing protein orientation on citrate-capped gold nanoparticles
64	Sunirmala Sahoo	Indian Institute of Science Education and Research Berhampur	Biophysical characterization of RelA-p52 NF-kB dimer – a link between the canonical and the non-canonical NF-kB pathway
65	Takahiro Kimura	Tohoku University	Single-molecule FRET investigation on the long-range contact formation in the folding of a gRNA granule of SARS-CoV-2
66	Tanaya Chatterjee	Bose Institute	The role of isoaspartic acid residues at different positions in the fibrillation of amyloid beta peptides and its inhibition by protein-L-isoaspartyl methyltransferase (PIMT)
67	Teena	Indian Institute of Technology Delhi	Biophysical Characterization and Interaction study of WhiB6 protein of Mycobacterium tuberculosis with espA
68	Trishita Banerjee	Advanced Centre for Treatment, Research and Education in Cancer (ACTREC), Tata Memorial Centre	Understanding the structural and functional mechanisms underlying the dynamic regulation of Pyruvate Kinase Muscle Isoform 2 (PKM2) in cancer
69	Varsha Shaji	Rajiv Gandhi Centre for Biotechnology, Thiruvananthapuram	Tuning Geometry and Functionality of α -Helical Nanopores through Site-Specific Incorporation of Natural and Unnatural Amino Acids
70	Hindol Chatterjee	IISER Kolkata	Unraveling Transition Path and Membrane Topological Characteristics in Bacteriorhodopsin Fragment Folding Pathway Implying Artificial Intelligence