भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

Department of
BIOTECHNOLOGY

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Vision, Mission, and Values

Our ***vision*** is to foster a world-class teaching environment and state-of-the-art facilities for cutting-edge biotechnology research to drive an academic space that is dedicated to cultivating innovative opportunities and systemwide collaboration for discovery beyond boundaries.

Our ***mission*** is to accelerate as an outstanding educational hub with an equal emphasis on excellence in teaching, research, and community engagement. We are committed to the utmost professional and academic standards to ensure intellectual excellence and to create a global impact by transmitting advanced knowledge.

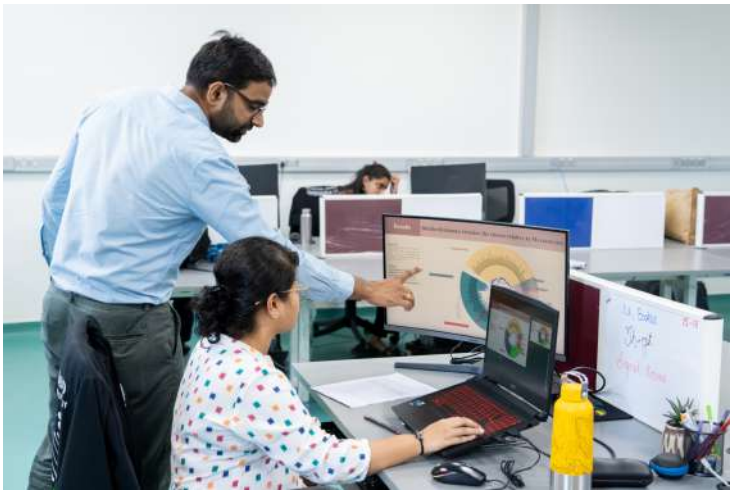
We aspire to ***value*** the highest academic and professional integrity, scientific ethics, and excellence in teaching and research to realize the full potential of biotechnology. We promote equality and empower our students, staff, and faculty to achieve intellectual rigor, academic leadership, and global recognition to best serve the nation and society.

Message from the HOD

Since the biotechnology department started its journey in 2010, the department has been striving for excellence in teaching and research. We have been continuously acquiring new capabilities and producing brilliant future scientists. We recently moved to our newly constructed state-of-the-art building in 2022, which is in the shape of a chromosome, further asserting our commitment to excellence. We have 15 world-class research laboratories and a dedicated teaching laboratory for students. The department offers B.Tech. in Biotechnology and Bioinformatics, M.Tech. in Medical Biotechnology, and Ph.D. in various Biotechnology and allied multidisciplinary areas at the forefront. Over the years, our uniquely formulated and tailored academic programs have attracted the best students. The total number of students in our department is currently 104. Our curriculum provides multifaceted opportunities to the students, including exposure to industrial problems so that we can address critical challenges not only faced by society but also industries which is the first and foremost requirement for “AatmaNirbhar Bharat”. We also have a unique biannual hands-on lab training, an out-reach programme, for researchers or students from Indian universities and institutes, and industrial professionals who want to enhance their wet-lab or computational biology research skills.

We are noted for our 15 excellent faculty members with varied expertise, trained in India and abroad. This brochure provides an overview of our department. I also invite you to learn more about the department faculty, research facilities, latest announcements and developments at https://biotech.iith.ac.in/.

Rajakumara Eerappa, PhD
Head, Department of Biotechnology
Associate Professor
Macromolecular Structural Biology Group




Nikon

Our Department

Hyderabad, the capital city of Telangana in India, has emerged as a prominent hub for the biotechnology industry, tackling a wide range of medical, industrial, and environmental challenges. In line with this growth, the Indian Institute of Technology Hyderabad established its Department of Biotechnology in 2010. Its mission is to cultivate a new generation of scientific leaders equipped with scientific rigor, critical thinking, ethics, and multitasking managerial skills to thrive in the rapidly evolving technology-driven industry and academia.

With 15 distinguished faculty members, the department excels in frontier areas of biotechnology research, including Structural Biology, Nanobiotechnology, Microbiology, Infection Biology, Cancer Biology, Computational Biology, and Bioprocess Technology. Working with various model systems such as bacteria, yeast, mouse, drosophila, zebrafish, and human cells, the research groups employ a range of molecular biology techniques and high-throughput omics-based platforms to address critical challenges in healthcare, agriculture, and environmental sustainability. The department boasts state-of-the-art laboratories equipped with advanced technologies and instrumentation, providing students and researchers with the necessary resources to conduct cutting-edge research.

While research takes center stage, the department also emphasizes high-quality teaching to nurture the next generation of biotechnologists. It offers undergraduate (B.Tech. in Biotechnology and Bioinformatics), postgraduate (M.Tech. in Medical Biotechnology), and doctoral programs (Biotechnology) that provide students with a solid foundation in biotechnology and its applications. The curriculum seamlessly integrates theoretical knowledge with practical training, enabling students to develop critical thinking, analytical skills, and a profound understanding of the subject matter. This research-centric approach cultivates a culture of inquiry and innovation, preparing students for successful careers in academia, industry, or entrepreneurship.

In addition to research and teaching, the department actively collaborates with industry partners, government organizations, and national/international institutions. These collaborations facilitate the exchange of knowledge, technology transfer, and the translation of research findings into real-world applications.

In the coming years, through its commitment to research excellence, quality teaching, and collaborative efforts, the Department of Biotechnology at IIT Hyderabad aims to play a pivotal role in advancing the biotechnology field and nurturing the next generation of biotechnologists.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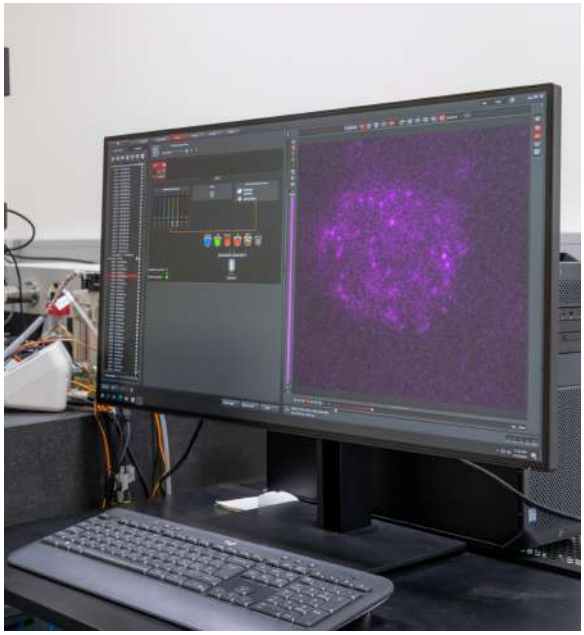


Courses Offered

B.Tech (Bioinformatics and Biotechnology)

Course Objectives: Develop a foundation for Biotechnology and Bioinformatics in young minds and inculcate interest by showing real-life challenges that can be addressed by biotechnology and bioinformatics. It is the first course among all the IITs that places equal emphasis on both experimental and computational aspects of biological sciences.

Duration: 4 years (8 semesters)

Eligibility Criteria: Based on JEE

Admission procedure: through JEE advanced
Features: 57 credits of core courses, 36 credits of elective courses, 5 credits of soft skill courses, 20 credits of practicals, and 6 credits of internship/departmental projects.

M.Tech (Medical Biotechnology) (admission through GATE or self-sponsored)

Course Objectives: Inculcate interest in the subject by nurturing a fundamental understanding of biological processes/phenomena and their medical applications, hands-on training with cutting-edge technologies, and effective science writing, presentation, and communication skills. This program makes the students ready to excel in academia/industry.

Duration: 2 years (4 semesters)

Eligibility Criteria: (through GATE) B.Tech/B.E./M.Sc. in any area of life sciences/M.Pharm, with a valid GATE score (in BT or XL). IIT B.Tech graduates with a CGPA of 8 or above without a GATE score are eligible to apply.
(self-sponsored) B.Tech/B.E./M.Sc. in any area of life sciences/M.Pharm with a CGPA of 7 and above (GATE score not required).

Admission procedure: (through GATE) based on GATE score through COAP, (self-sponsored) Online interviews

Features: 26 credits of coursework (first two semesters), 24 credits of research thesis (last two semesters), exposure to scientific writing, presentation, and communication, a stipend of Rs. 12,500 per month for MoE students

Ph.D. (Biotechnology)

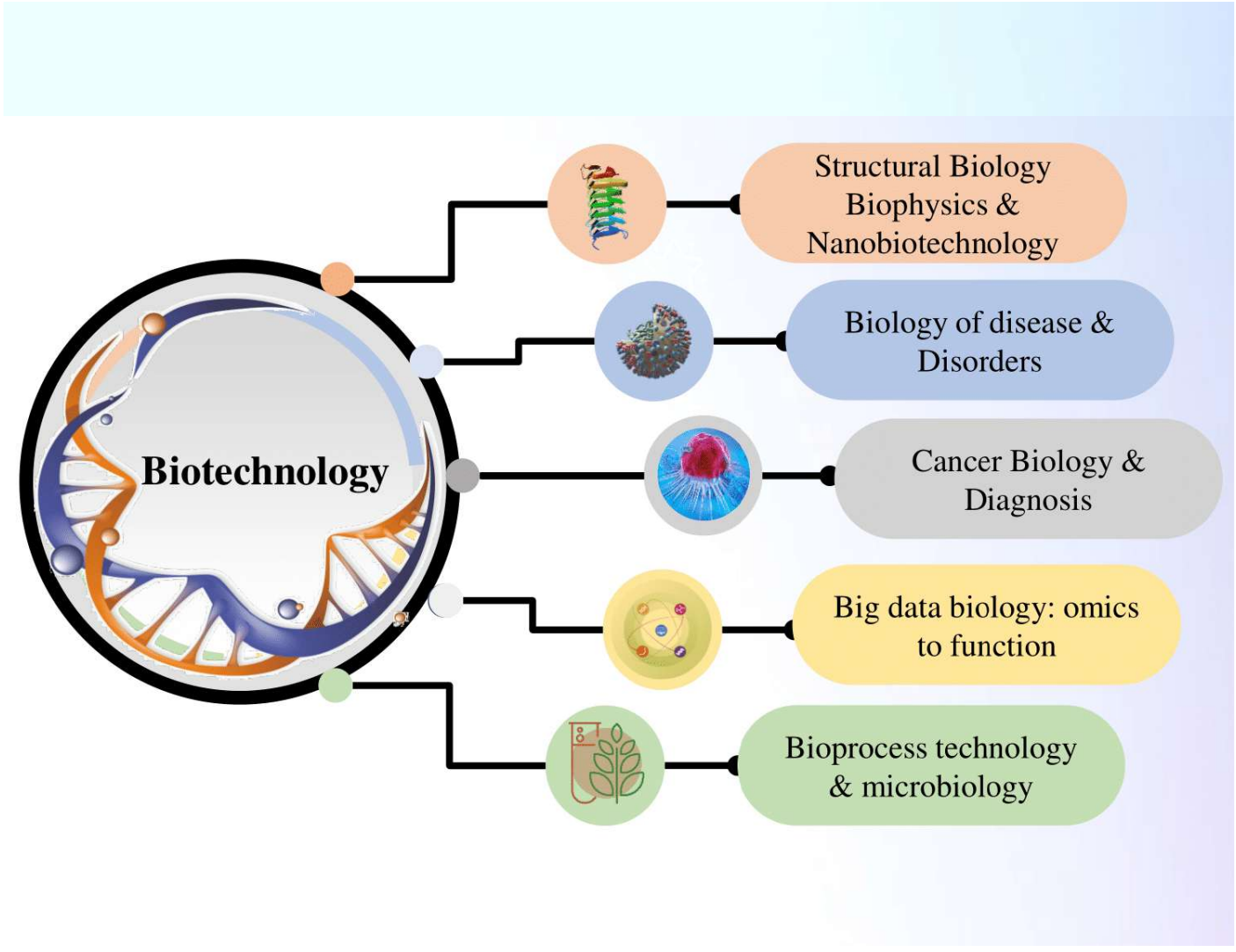
Course Objectives: Our research-intensive Ph.D. program intends to develop future leaders of biotechnology by developing skills such as independent and intellectual thinking, interdisciplinary research, scientific writing, presentation, communication, and science ethics. Students are given independent research projects on frontier areas of biotechnology and they are taught cutting-edge technologies to address biological problems.

Duration: 5 years

Eligibility Criteria: B.Tech/B.E./M.Tech/M.Sc./M.E. in any area of life sciences, M.Pharm, MBBS, MD/MS. A valid national-level JRF (CSIR-JRF/UGC-JFR/DBT-JRF (category I), DST-INSPIRE) or GATE qualification is required for B.Tech/B.E./M.Sc.

Admission procedure: Interview (twice a year, in June and December)

Features: 12-24 credits of coursework, publications in international peer-reviewed journals, patents, presentations at national and international conferences, skill development workshops, opportunities for Joint Doctoral Programs (JDPs) with renowned foreign universities, and Interdisciplinary Ph.D. programs.


Biotechnology
Structural Biology Biophysics & Nanobiotechnology
Biology of disease & Disorders
Cancer Biology & Diagnosis
Big data biology: omics to function
Bioprocess technology & microbiology

Faculty Broad Theme Areas

	Structural Biology, Biophysics and Nanobiotechnology	Biology of Diseases and Disorders	Cancer Biology and Diagnosis	Big Data Biology: Omics to function	Bioprocess Technology and Microbiology
Abhishek Subramanian		✓		✓	
Althuri Avanthi					✓
Anamika Bhargava	✓	✓	✓		
Anindya Roy			✓		✓
Ashish Misra		✓	✓	✓	
Basant Kumar Patel	✓	✓			
Gaurav Sharma				✓	✓
Gunjan Mehta	✓	✓	✓		✓
Himanshu Joshi	✓				
Indranil Malik	✓	✓			
NK Raghavendra		✓			
Rahul Kumar		✓	✓	✓	
Rajakumara Eerappa	✓	✓	✓		
Sandipan Ray		✓	✓	✓	
Thenmalarchelvi Rathinavelan	✓	✓		✓	

BROAD THEME AREAS

Rajkumara Eerappa

Basant Kumar Patel

Gunjan Mehta

Thenmalarchelvi Rathinavelan

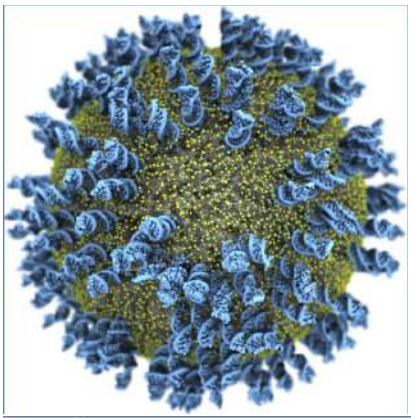
Himanshu Joshi

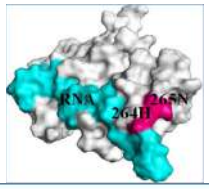
Anamika Bhargava

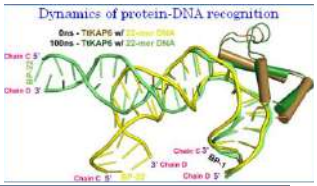
Indranil Malik

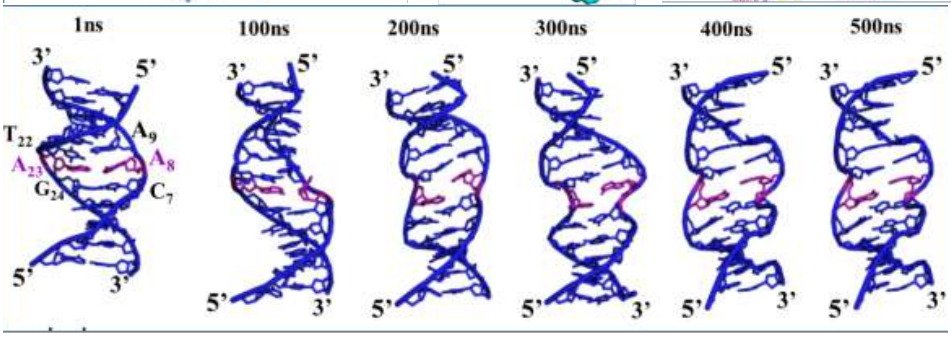
Structural Biology, Biophysics and Nanobiotechnology

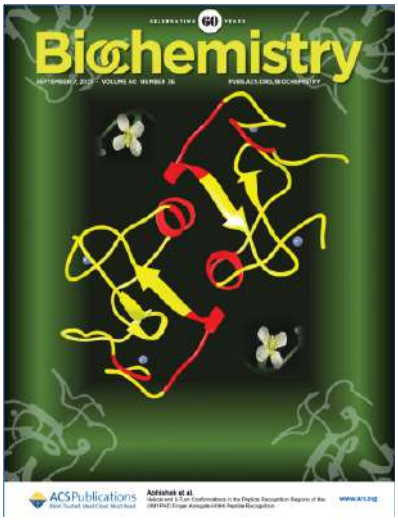
- Structural studies of epigenetic marks reader proteins
- Electrophysiological measurements through voltage-gated calcium channels
- Harnessing the high-performance computing (HPC) to decipher the nanoscale structure and dynamics of self-assembled synthetic nano-biosystems.
- Developing computational models to illustrate the physics of living cells and the interaction of nanomaterials with the biological matter.
- RRM1-2 domain structure of the TDP-43 protein showing predicted Zinc binding amino acids in pink.
- AFM image of amyloid-like aggregates of E540V familial mutant bearing Fibrinogen A-alpha chain fragment protein.











BROAD THEME AREAS

Anamika Bhargava

Anindya Roy

Ashish Misra

Rahul Kumar

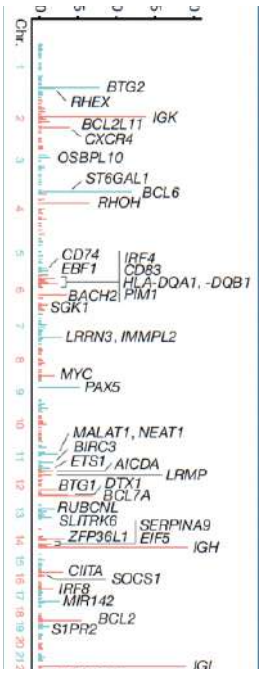
Gunjan Mehta

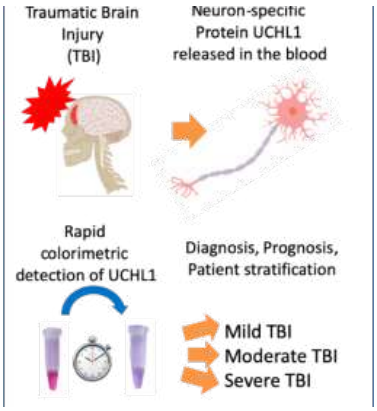
Sandipan Ray

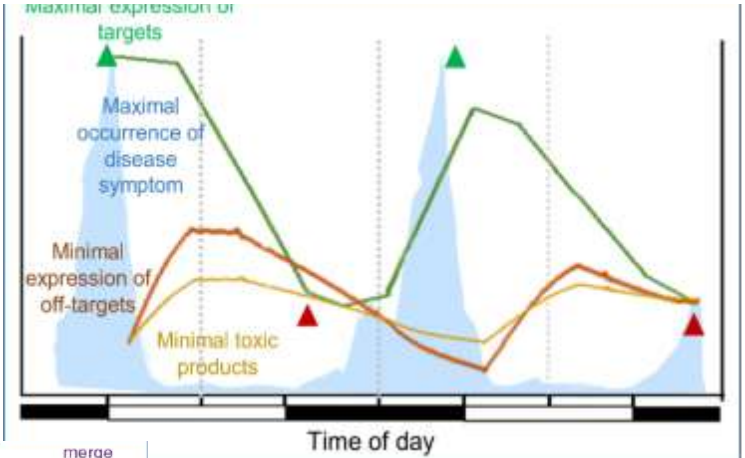
Rajkumara Eerappa

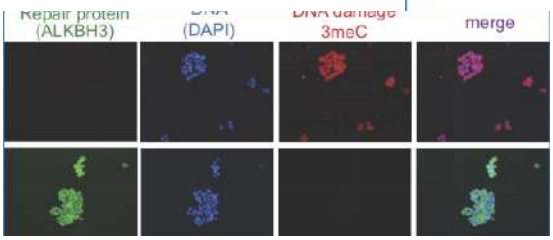
Cancer Biology and Diagnosis

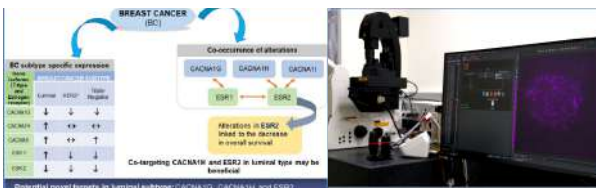
- A reliable, rapid, cost-effective method for detection of TBI biomarker UCHL1
- Characterization of regulation of cancer drug targets PARP1 and PARP2
- Ion-channel dysfunction in breast cancer
- Development of zebrafish xenotransplantation models for the analysis of breast cancer subtypes
- Identified details of the enzymes engaged in removing the alkyl groups from the modified DNA bases in cancer cells
- Chromatin remodelers play essential roles during meiosis.
- Dosing time dependency of anticancer drugs











BROAD THEME AREAS

Basant Kumar Patel

Gunjan Mehta

Thenmalarchelvi Rathinavelan

NK Raghavendra

Sandipan Ray

Ashish Misra

Abhishek.S

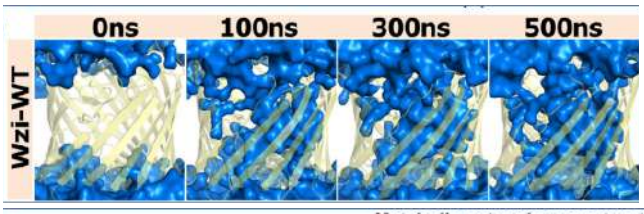
Rahul Kumar

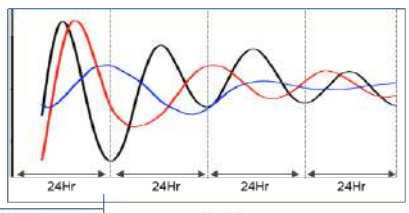
Anamika Bhargava

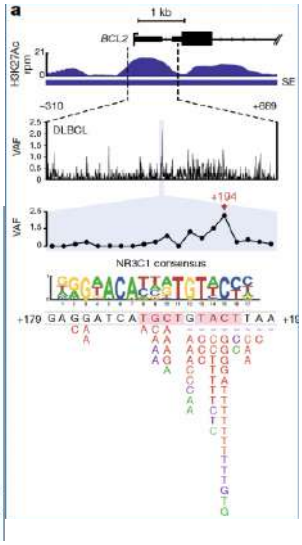
Rajkumara Eerappa

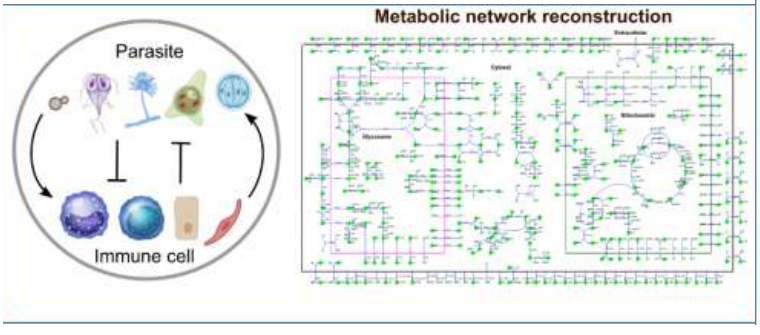
Biology of Diseases and Disorders

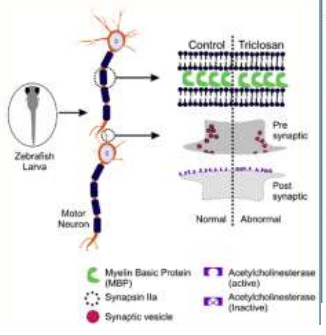
- Designing and evaluation of small molecule phosphodiesterase inhibitors to modulate sperm competence for IVF
- Mechanisms of diseases/toxicity caused by chemicals and pollutants
- Use of zebrafish model for toxicity and biocompatibility studies
- Computational reconstructions of parasites & host immune cell metabolism for deciphering infection-induced metabolic changes
- In vitro liquid-Liquid phase separation of Alexa fluor-labelled A315T familial mutation-bearing fragment of TDP-43 protein implicated in ALS disease.
- Underpinning the mechanistic basis of disease pathology
- Circadian regulation and irregularities in cardiovascular disease patients











BROAD THEME AREAS

Rahul Kumar

Gaurav Sharma

Abhishek Subramanian

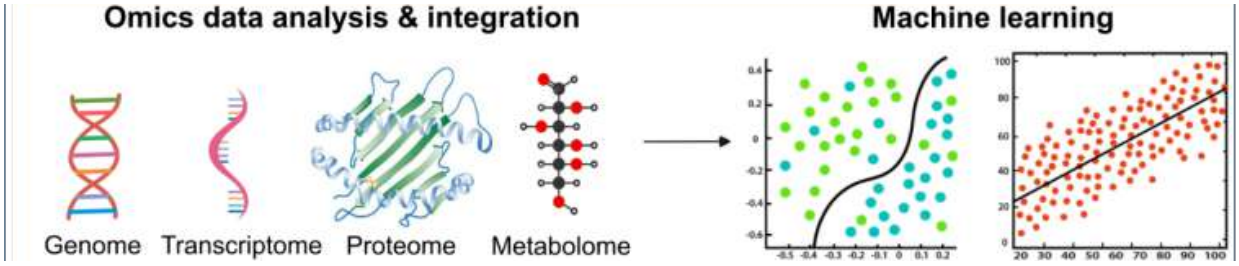
Sandipan Ray

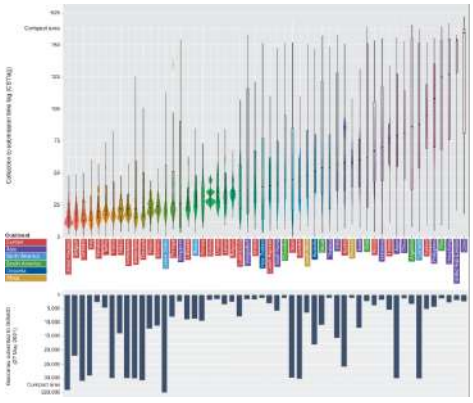
Thenmalarchelvi Rathinavelan

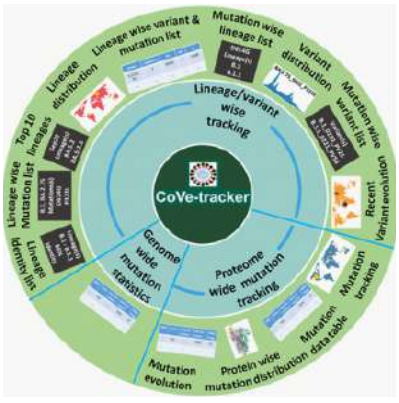
Ashish Misra

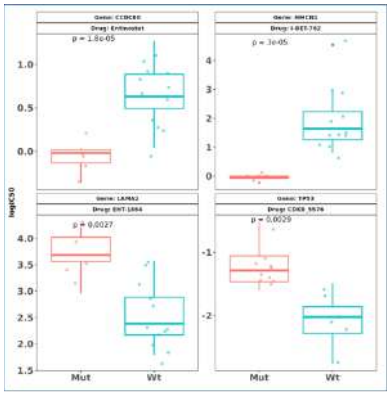
Big Data Biology: Omics to function

- Omics data analysis, integration and machine learning
- Gene regulatory network inference
- Developing AI/ML based tools to identify diagnostics and prognostic biomarkers of various cancer types using large volume of omics data.
- High-throughout pan kingdom bacterial genome analysis to understand their physiology, function and evolution
- High-throughput genome and metadata analysis of SARS-CoV-2 sequences
- Circadian regulations of kinome and signaling
- Development of zinc finger motif prediction tool and in silico diagnostic tools for Gram-negative bacterial serovar prediction
- Genomic and transcriptomic profiling of Indian cancer patients for personalized medicine









BROAD THEME AREAS

Althuri Avanthi

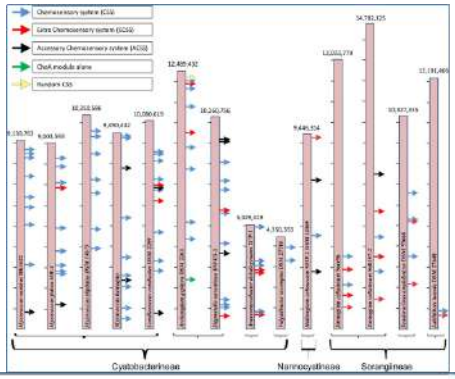
Gaurav Sharma

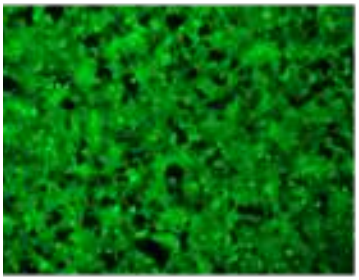
Gunjan Mehta

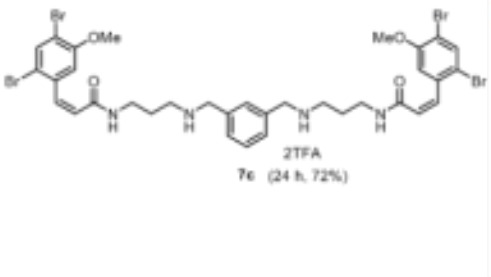
Anindya Roy

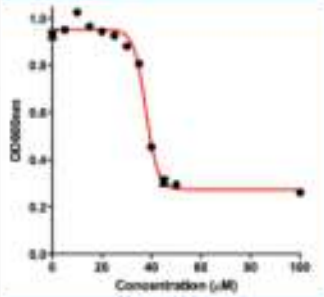
Bioprocess Technology and Microbiology

- Development of waste valorization technologies for the production of Biofuels, Biochemicals, and Biomaterials
- Exploring ways to transform linear economy to circular economy through multi-product approach
- Identification and taxonomic classification of novel bacterial organisms from diverse niche followed by their comparative genomic studies
- Identification of ML0190 as the Mycobacterium leprae DNA repair protein by genetic complementation
- Comparative genomics and phylogenetic approaches to understand the physiology of microbes









Abhishek Subramanian

Assistant Professor

Email: abhisheks@bt.iith.ac.in
Lab website: https://sites.google.com/bt.iith.ac.in/comp-bio-abhishek

PhD from CSIR - National Chemical Laboratory, Pune, India

- Computational Systems & Network Biology
- Omics data analysis & bioinformatics
- Metabolism & gene regulation
- Mathematical, statistical modelling and machine learning
- Parasitology and immunology

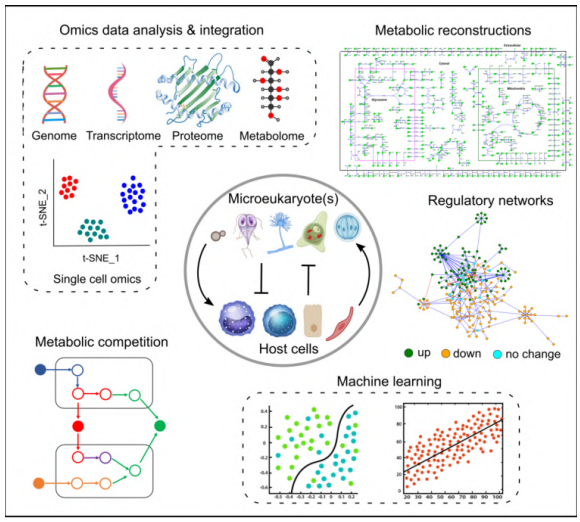
Our group employs various bioinformatics and computational techniques to develop in-silico models that can integrate multi-omics data for the inference, analysis and semi-automated development of networks for discovering novel biological mechanisms.

Our group is specifically interested in understanding the "systems biology" of infections from both the host and parasite perspectives. Our tangible research outputs include the development of computational models, pipelines, software, web servers and databases in the above context. Our projects currently focus on -

1. Development of novel, semi-automated metabolic reconstructions of parasitic fungi, protozoa and amoebae: Here, we develop genome-scale metabolic network models (GEMs) by annotation of metabolic enzymes, reaction, metabolite and subcellular locations and use the reaction-metabolite network for the prediction of condition-specific metabolic reaction fluxes and their biochemical purposes.

2. Gene regulatory / signaling pathway networks of host immune cells during parasitic infection: The interaction of innate immune cell receptors with pathogen-specific molecular patterns trigger differentially-timed transcriptional regulatory responses which can reprogram metabolism in innate immune cells. We aim to develop machine – learning models using omics data for the prediction of such genome-scale transcriptional regulatory events.

3. Modeling the mechanistic influence of transcriptional regulation interactions on innate immunometabolism: Predicted regulatory mechanisms along with differential transcriptomics changes can be integrated with existing generic human metabolic models to computationally model the influence of transcriptional regulation on innate immune cell metabolic behaviour.



PUBLICATIONS

Abhishek Subramanian, Pooya Zakeri, Mira Mousa, Halima Alnaqbi et al.
Angiogenesis goes computational – the future way forward to discover new angiogenic targets?
2022
Computational and Structural Biotechnology Journal
https://doi.org/10.1016/j.csbj.2022.09.019

Katerina Rohlenova, Jermaine Goveia, Melissa García-Caballero, Abhishek Subramanian et al
Single-Cell RNA Sequencing Maps Endothelial Metabolic Plasticity in Pathological Angiogenesis
2020
Cell Metabolism
https://doi.org/10.1016/j.cmet.2020.03.009

Abhishek Subramanian, Ram Rup Sarkar
Evolutionary Perspectives of Genotype–Phenotype Factors in Leishmania Metabolism
2018
Journal of Molecular Evolution
https://doi.org/10.1007/s00239-018-9857-5

Abhishek Subramanian, Ram Rup Sarkar
Revealing the mystery of metabolic adaptations using a genome scale model of Leishmania infantum
2017
Scientific Reports
https://doi.org/10.1038/s41598-017-10743-x

Sutanu Nandi, Abhishek Subramanian, Ram Rup Sarkar
An integrative machine learning strategy for improved prediction of essential genes in Escherichia coli metabolism using flux- coupled features
2017
Molecular BioSystems
https://doi.org/10.1039/C7MB00234C

COLLABORATIONS

Academic

1. Prof. Peter Carmeliet, VIB-KU Leuven Center for Cancer Biology, Leuven, Belgium
2. Dr. Ram Rup Sarkar, CSIR – National Chemical Laboratory, Pune, India

PATENTS

1. Ram Rup Sarkar, Rupa Bhowmick, Abhishek Subramanian, Method of Identification of Combinatorial Enzymatic Reaction Targets in Glioblastoma Specific Metabolic Network, US Patent App. 15/779,798, 2018 (Patent Submitted)

AWARDS

1. DBT - Ramalingaswamy Re-entry Fellowship 2021-22 from the Department of Biotechnology (DBT), Government of India
2. Keerthi Sangoram Memorial Endowment Award for Best Research Scholar in the area of Biological Sciences by CSIR-NCL Research Foundation, India
3. Award for the Best Poster at the 1st IBSE International Symposium held at Indian Institute of Technology (IIT), Madras, India
4. ISCB/InCOB Travel Grant obtained for attending the 15th International Conference on Bioinformatics (InCOB), Matrix Biopolis, Singapore

Althuri Avanthi

Assistant Professor

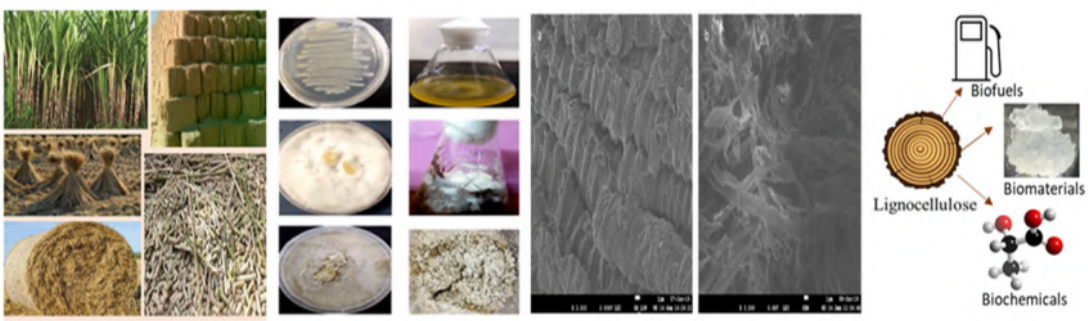
Email: a.avanthi@bt.iith
Lab website: https://sites.google.com/bt.iith.ac.in/integratedbioprocesstechnology/home

PhD from IIT Kharagpur

- Biofuels, Biochemicals, and Biomaterials
- Bioprocess technology, Fermentation, and Downstream processing
- Nanobiotechnology and Hydrothermal Liquefaction
- Waste valorisation and Circular economy

Our Lab is inclined towards developing low-cost green technologies with possible applications in Agricultural, Medical, and Environmental sectors. We are exploring ways to transform linear economy to circular economy through multi-product approach.

The lab is focused on unravelling the challenges in lignocellulosic biomass/ Agro-residue/ bio-genic waste valorisation. These are potential feedstocks for synthesis of biochemicals, biofuels and biomaterials that are sustainable alternatives to the conventional synthetic equivalents. This approach can reduce the dependency on non-renewable fossil resources for meeting the burgeoning market demand and thus can effectively minimize virgin resource depletion. Our goal is to utilize diverse bio-genic wastes and process the recovered or extracted biomolecules to commercially imperative deliverables. Lignin is a vital component which gives stability towards biodegradation to lignocellulose biomass; this property of lignin is exploited to design hydrogels with applications in the food packaging. Along with lignin, the research has been broadened to recover cellulose and hemicellulose and process them into bioproducts like aerogels and yeast oil, with applications in several sectors such as biofuel, cosmetic, biomedical, environment, agriculture etc. Besides recovering the polymers from feedstocks, our research has been extended to the extraction of mono-saccharomates followed by bioconversion into Lactic acid using one-pot microbial fermentation and subsequent polymerization into Polylactic acid (PLA). The research on PLA has been further advanced to design a biodegradable non-woven material. Our research team also deals with contemporary concepts like nanobiotechnology in biogenic waste pre-treatment, self-cycling fermentation, and circular economy and industrial symbiosis.



PUBLICATIONS

Avanthi Althuri, S. Venkata Mohan
2022
Emerging innovations for sustainable production of bioethanol and other mercantile products from circular economy perspective
Bioresource Technology
https://doi.org/10.1016/j.biortech.2022.128013

Avanthi Althuri, S. Venkata Mohan
2020
Sequential and consolidated bioprocessing of biogenic municipal solid waste: a strategic pairing of thermophilic anaerobe and mesophilic microaerobe for ethanol production
Bioresource Technology
https://doi.org/10.1016/j.biortech.2020.123260

Avanthi Althuri, Jincy Mathew, Raveendran Sindhu, Rintu Banerjee, Ashok Pandey, Parameswaran Binod
2013
Microbial synthesis of poly-3- hydroxybutyrate and its application as targeted drug delivery vehicle
Bioresource Technology
https://doi.org/10.1016/j.biortech.2013.01.106

Avanthi A and Banerjee R
2017
Separate and simultaneous saccharification and fermentation of pretreated mixture of lignocellulosic biomass for ethanol production
Biofuels
https://doi.org/10.1080/17597269.2017.1409059

Avanthi A and Banerjee R
2016
A strategic laccase mediated lignin degradation of lignocellulosic feedstocks for ethanol production
Industrial Crops and Products
https://doi.org/10.1016/j.indcrop.2016.08.009

COLLABORATIONS

Academic

1. Dr S Venkata Mohan, Chief Scientist, CSIR-Indian Institute of Chemical Technology, Hyderabad
2. Dr Binod Parameswaran, Principal Scientist, CSIR – National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram, Kerela
3. Dr. Knawang Chhunji Sherpa, Scientist, CSIR – National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram, Kerela
4. Dr. Gujjala Lohit Kumar Srinivas, Assistant Professor, NIT Rourkela
5. Dr. Shyam Krishna, Research Professor, Kyung Hee University, Republic of Korea

AWARDS

1. Invited Reviewer for Bioresource Technology Journal, Elsevier (Impact factor: 11.88), Microbial cell factories, Springer Nature (Impact factor: 6.352) and Journal of Environmental Management, Elsevier (Impact factor: 5.84).
2. Associate Fellow of Telangana Academy of Sciences (TAS), Telangana (2019)
3. CSIR-Nehru Science Postdoctoral Research Fellowship (2018-2021)
4. Moderator (Thematic session- Agriculture and Food Processing) & host (award ceremony) for SCO – 1st Young Scientists Conclave, sponsored by Department of Science and Technology, Government of India and organized by CSIR-IICT, Hyderabad
5. Received two international travel grants for attending bioenergy conferences at Rome, Italy and Khon Kaen, Thailand sponsored by IIT Kharagpur.

PATENTS

1. Yellow laccase mediated delignificati on of lignocellulo sic biomass
   Banerjee R, Ghangrekar MM, Rajak RC, Chintagunta AD, Althuri A, Srinivas GLK, Sherpa KC, and Kumar S
   201631005954
   20.02.2016
   India

Anamika Bhargava

Associate Professor

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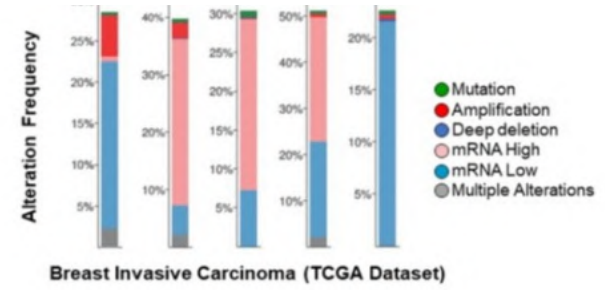
Lab website: https://csl.biotech.iith.ac.in/

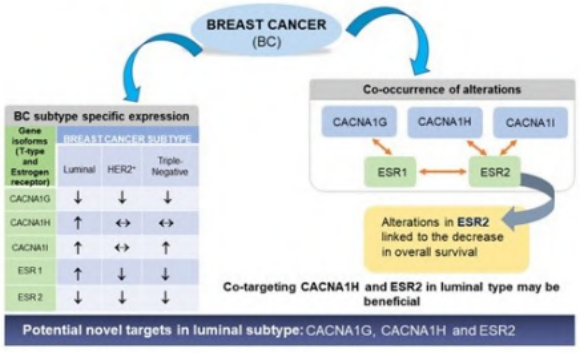
PhD from Medical University Innsbruck, Austria

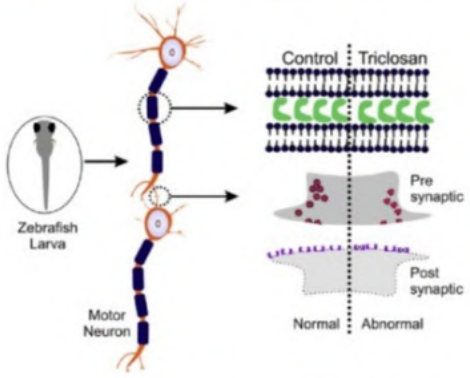
- Voltage-gated calcium channels in health and disease
- Ion channels in cancer
- Cell signalling through ion channels
- Investigation of disease and toxicity mechanisms using zebrafish model
- Development of zebrafish models of xenotransplantation

Our lab is interested in studying cell signalling through membrane receptors such as ion channels and other proteins interacting with ion channels. We use in-vitro and in-vivo models to investigate receptors in health and disease.

Our lab works at the interface of heath and disease. We use molecular biology, protein chemistry, cell culture and specialized techniques such as calcium imaging, patch-clamp electrophysiology and advanced microscopy to understand how membrane receptors work and how they contribute to diseases where they are dysfunctional. We aim to understand the importance of ion channel receptors in maintaining health and balance of organs such as heart, brain, etc. and how their dysfunction may be detrimental for humans. Currently we are studying the role of T-type calcium channels in triple negative breast cancer and their interaction with estrogen receptors. We are interested to observe the expression of calcium channels in Indian breast cancer patients and understand whether calcium channels can be drug targets in breast cancer. As an alternate to rodent models, we have established zebrafish animal model in our lab. We are interested in investigating pathological mechanisms using zebrafish animal model including breast cancer pathogenesis in zebrafish xenotransplantation models.







PUBLICATIONS

M Agarwal, A Sharma, A Kagoo R, A Bhargava
Interactions between genes altered during cardiotoxicity and neurotoxicity in zebrafish revealed using induced network modules analysis
2023
Scientific reports
https://www.nature.com/articles/s41598-023-33145-8

Shwetha Sekar, Yashashwini Subbamanda, Narasimha Pullaguri, Ankush Sharma, Chittaranjan Sahu, Rahul Kumar, Anamika Bhargava.
Isoform-specific expression of T-type voltage-gated calcium channels and estrogen receptors in breast cancer reveals specific isoforms that may be potential targets
2022
Current Research in Biotechnology
https://www.sciencedirect.com/science/article/pii/S2590262822000375?via%3Dihub

Pullaguri, N., Grover, P., Abhishek, S., Rajakumara, E., Bhargava, Y., Bhargava, A.
Triclosan affects motor function in zebrafish larva by inhibiting ache and syn2a genes
2020
Chemosphere
https://www.sciencedirect.com/science/article/abs/pii/S0045653520331271?via%3Dihub

Gaur H, Pullaguri N, Nema S, Purushothaman S, Bhargava Y, Bhargava A
An Open-Source Method for Cardiac-Rhythm Estimation in Untethered Zebrafish Larvae
2018
Zebrafish
https://www.liebertpub.com/doi/10.1089/zeb.2017.1545?url_ver=Z39.88-2003&rfr_id=ori%3Arid%3Acrossref.org&rfr_dat=cr_pub++0pubmed

Anamika Bhargava, Xianming Lin, Pavel Novak, Kinneri Mehta, Yuri Korchev, Mario Delmar and Julia Gorelik.
Super-resolution scanning patch-clamp reveals clustering of functional ion channels in the adult ventricular myocyte
2013
Circulation research
https://www.ahajournals.org/doi/10.1161/CIRCRESAHA.111.300445?url_ver=Z39.88-2003&rfr_id=ori:rid:crossref.org&rfr_dat=cr_pub%20%200pubmed

COLLABORATIONS

Academic

1. Prof. Julia Gorelik, Imperial College London, London
2. Dr Yogesh Bhargava, Dr Hari Singh Gour Central University Sagar, M.P India
3. Dr Shishir Kumar, Indian Institute of Technology, Hyderabad
4. Dr Swapna Jilla, Senior consultant, and Head of the Department of Radiation oncology, Mallareddy Narayana multispeciality hospital, Hyderabad
5. Dr Andres Maturana, Nagoya University, Japan

AWARDS

1. Invited Review Editor, Frontiers of physiology: cardiac electrophysiology (2021).
2. Early Career Research Award, Science & Engineering Research Board (SERB), Department of Science & Technology (DST) (2018).
3. Outstanding women in science award by Venus international foundation (2017).
4. Honorary research associateship, Imperial College London (2016).
5. Lewis MacDonald Award for best proposal, Heart and Stroke Foundation of BC and Yukon, Canada (2009).

Anindya Roy

Professor

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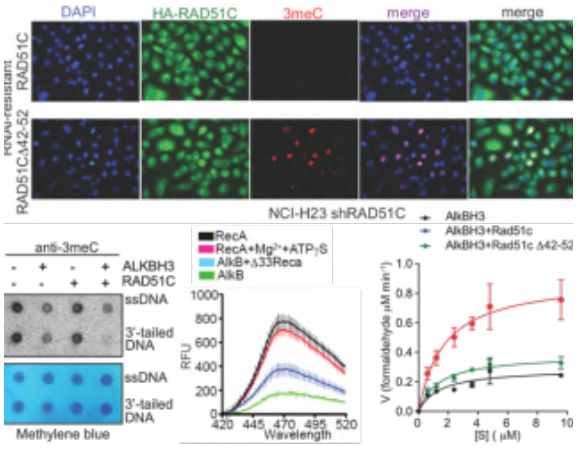
Lab website: https://sites.google.com/iith.ac.in/arlab

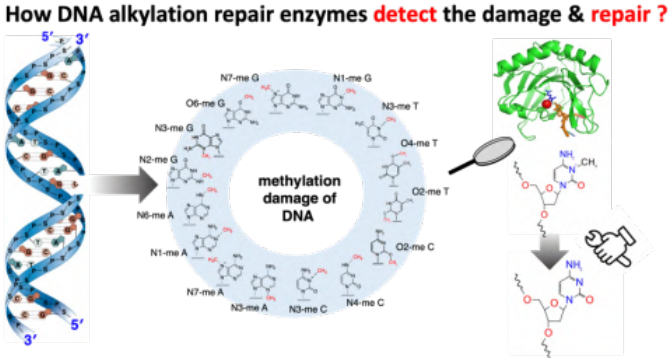
PhD from Indian Institute of Science, Bangalore

- Molecular characterization of DNA alkylation damage repair enzymes
- Role of DNA alkylation in cancer, autoimmune and inflammatory diseases

My lab is interested in understanding molecular mechanisms underlying DNA alkylation damages and the enzymes involved in repairing this damages.

The lab has a long-standing interest in DNA alkylation modifications and their repair. While some of the key enzymes that repair these modifications are known, their relationship to genome integrity is less clear. We previously established roles for E coli AlkB, S cerevisiae Tpa1 and human ALKBH3 and ALKBH5 DNA demethylases in DNA repair (Shivange et al, JBC, 2014; Shivange et al, NAR, 2016, Nigam et al BBRC 2018, Akual et al, BBRC, 2021). This led us to the discovery of a RAD51C-dependent mechanism that recruits ALKBH3 demethylase to the DNA (Mohan et al, NAR, 2019). We now have several lines of investigation related to this pathway: What are the factors that may regulate this pathway? Can this pathway be targeted for cancer therapy? How this pathway is connected to other nucleic acid metabolism pathways? What is the effect of this pathway on inflammation and innate immune pathways? Mice deficient in DNA alkylation repair enzymes are highly susceptible to acute and systemic inflammation. We are also studying the molecular mechanism behind it. We have also broadened our studies on DNA alkylation repair enzymes to development of highly sensitive quantitative approaches to analyse DNA alkylation repair rates. We aim to apply these methods in discovering new inhibitors for the DNA alkylation repair enzymes. To this end, we found some novel lead molecules (Nigam et al, CBDD, 2021; Negi et al, OBC, 2022) and our lab is researching to discover more such inhibitor molecules.





PUBLICATIONS

G. Shivange, N. Kodipelli, M. Monisha, R. Anindya
A role for Saccharomyces cerevisiae Tpa1 protein in direct alkylation repair
2014
Journal of Biological Chemistry
www.sciencedirect.com/science/article/pii/S002192582057988X

G. Shivange, M. Monisha, R. Nigam, N. Kodipelli, R. Anindya
RecA stimulates AlkB-mediated direct repair of DNA adducts
2016
Nucleic Acid Research
www.academic.oup.com/nar/article/44/18/8754/2468346

M. Mohan, D. Akula, A. Dhillon, A. Goyal, R. Anindya
Human RAD51 paralogue RAD51C fosters repair of alkylated DNA by interacting with the ALKBH3 demethylase
2019
Nucleic Acid Research
www.academic.oup.com/nar/article/47/22/11729/5603225

COLLABORATIONS

Academic

1. Dr G. P. Singh, AIIMS, New Delhi
2. Dr Prolay Das, IIT Patna, Patna, Bihar
3. Dr Arun Goyal, IIT Guwahati, Guwahati, Assam
4. Dr F. A. Khan, IIT Hyderabad, Hyderabad, Telangana
5. Dr Timothy O'Connor, City of Hope Medical Centre, Duarte, CA, USA

Industrial

1. Achira labs, Bangalore
2. miBiome Therapeutics, Mumbai

AWARDS

1. Gandhian Young Technological Innovation (GYTI) Mentor Award (2015)
2. Excellence in Teaching Award, IIT Hyderabad (2015)
3. Innovative Young Biotechnologist Award (IYBA), Govt. of India (2008)

PATENTS

1. Composition, method and kit for rapid risk stratification of traumatic brain injury, PCT/201741042270, Published

Dr. Ashish Misra

Assistant Professor

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Lab website: https://cgrblab.bt.iith.ac.in/index.html

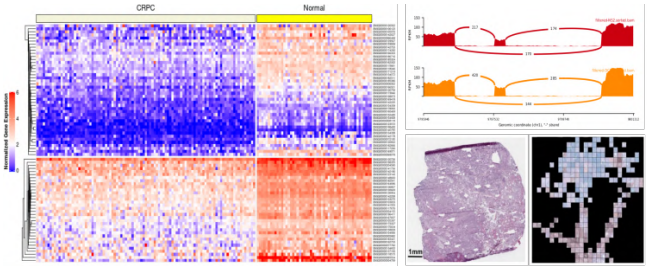
PhD from Molecular Biophysics Unit, Indian Institute of Science, Bengaluru, India

- Pre-clinical validation of tissue-based prognostic and predictive biomarkers in therapy resistant Indian prostate cancer patients.
- Identification and pre-clinical validation of therapeutically targetable oncogenic drivers of castration-resistant prostate cancer
- Constructing the Genomic and Transcriptomic landscape of Indian pediatric B-cell Acute Lymphoblastic Leukemia patients to identify novel prognostic and therapeutic targets.
- Understanding the role of Long non-coding RNAs and alternative splicing in cancer progression

Employing a constellation of tools and techniques, our overarching goal is to identify and develop clinically actionable solutions for treatment of Indian cancer patients.

Castration-resistant prostate cancer (CRPC) is an aggressive and currently incurable form of prostate cancer with an extremely high mortality rate. Despite remarkable improvements in patient survival rate with next generation androgen-receptor signalling inhibitors such as abiraterone and enzalutamide, almost all patients develop drug resistance and eventually die from the disease within a short span of time. In India, 1.4 million men are diagnosed with Prostate cancer annually - of which 85% cases are stage IV CRPC cancer patients. The numbers have increased to 1.9 million in 2020 and are expected to get doubled by 2030. Thus, there is an urgent need to comprehensively understand the mechanisms of drug resistance and develop new approaches for overcoming such resistance. We employ a constellation of tools and methodologies to investigate the mechanisms regulating drug resistance, with the overarching aim of providing clinically actionable solutions for the treatment of the disease.

B-cell acute lymphoblastic leukemia (B-ALL) is characterized as pestiferous multiplication of nascent B-cell lymphocytes, which is very detrimental to the immune system, severely affecting both children and adults. Although, in past few decades, in well developed countries, the survival rate of pediatric patients with B-ALL has jumped to more than 90%, but intriguingly, developing countries like India, still report dismal cure and high relapse rate. The most common complications arising due to current chemotherapy treatment are drug induced cytotoxicity and late relapse due to which the mortality rate is still very high in India when compared to other developed countries. Therefore, targeting molecular pathways and drivers involved in B-ALL pathogenesis, in addition to conventional chemotherapy treatment, can assuage the existing treatment protocol available for B-ALL. Understanding the genomic and transcriptomic landscape of B-ALL is key to understanding the underlying reasons of relapse and developing personalised medicine. Evolving data on genome and transcriptome of pediatric B cell ALL indicates significant contributions from ethnic, racial, and geographical variations. Genomic and transcriptomic data on Indian paediatric B cell ALLs is presently lacking. In this study we aim to generate genomic and transcriptomic data of Indian pediatric B lymphoblastic leukemia using multimodal technological approach along with an attempt to identify the incidence of various genetic subgroups. Besides determining the incidences of various subgroups of B-cell ALL, the study will allow us to generate and evaluate genomic and transcriptomic profile of Indian patients with various genetic subgroups of B-cell ALL. Depending upon the incidence of novels subgroups, we expect to be able to detect and generate the RNA and DNA profile of common novel subgroups of B ALL in India and get an understanding of expression profiles of Indian B cell ALLs which will help identify novel targets for treatment of this complex disease and overcome drug resistance.



PUBLICATIONS

Kumbhakara S, Gupta P, Giri B, Karumbana KS, Muleya A, Misra A*, Maji S*.(* corresponding authors)
Photolability of NO in ruthenium nitrosyls with pentadentate ligand induces exceptional cytotoxicity towards VCaP, 22Rv1 and A549 cancer cells under therapeutic condition.
2022
Journal of Molecular Structure
https://doi.org/10.1016/j.molstruc.2022.133419

Karumbana KS, Raut R, Gupta P, Muleya A, Giri B, Kumbhakara S, Misra A*, Maji S*. (* corresponding authors)
Mononuclear cobalt(II) complexes with Polypyridyl Ligands: Synthesis, Characterization, DNA interactions and in vitro cytotoxicity towards human cancer cells.
2022
Journal of Inorganic Biochemistry
https://doi.org/10.1016/j.jinorgbio.2022.111866

Karumbana KS, Muleya A, Raut R, Gupta P, Giri B, Kumbhakara S, Misra A*, Maji S*.(* corresponding authors)
Mononuclear Co(II) polypyridyl complexes: synthesis, molecular structure, DNA binding/cleavage, radical scavenging, docking studies and anticancer activities.
2022
Dalton Transactions
https://doi.org/10.1039/D1DT04144D

Manohar K, Gupta RK, Gupta P, Saha D, S Gare, Sarkar R, Misra A, Giri L.
FDA approved L-type channel blocker Nifedipine reduces cell death in hypoxic A549 cells through modulation of mitochondrial calcium and superoxide generation
2021
Free Radical Biology & Medicine
https://doi.org/10.1016/j.freeradbiomed.2021.08.245

Giri B, Saini T, Kumbhakar S, Kalai Selvan K, Muleya A, Misra A*, Maji S*(* corresponding authors)
Near-IR Light-induced Photo release of nitric oxide (NO) on Ruthenium Nitrosyl Complexes: Electronic structure, reactivity aspects, and biological effects
2020
Dalton Transactions
https://doi.org/10.1039/D0DT01788D

COLLABORATIONS

Academic

1. Dr. Somnath Maji, Department of Chemistry, IIT Hyderabad
2. Dr. Suhanya Duraiswamy, Department of Chemical Engineering, IIT Hyderabad
3. Prof. Nishant Verma, Department of Pediatrics, King George Medical University, Lucknow
4. Prof. Ashutosh Kumar, Department of Biosciences and Bioengineering, IIT Bombay

Industrial

1. Dr. Vishal B Rao, Basavatarakam Indo American Cancer Hospital and Research Institute, Banjara Hills, Hyderabad
2. Dr. Shirisha Rani G, Hematology, Oncology and BMT, Rainbow Children's Hospital, Hyderabad

AWARDS

1. Review Editor- Frontiers in Genetics (2021-present)
2. Review Editor- Frontiers in Molecular Biosciences (2021-present)
3. Early Career Research Award, Science and Engineering Research Board (SERB)" 2018
4. Student fellowship from the organizers of 32nd FEBS conference held in Vienna, Austria (2007)
5. INSA fellowship for attending the 32nd FEBS conference in Vienna, Austria. (2007)

Basant Kumar Patel

Associate Professor

Phone: 91-40-23016151
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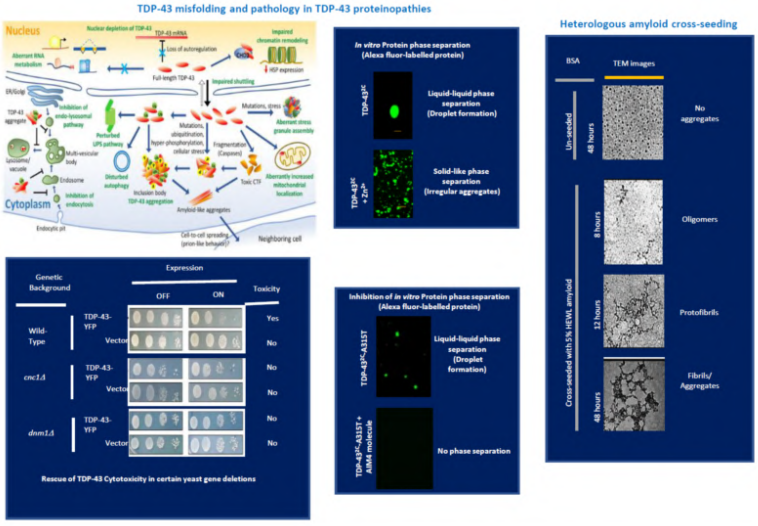
Lab website: https://sites.google.com/iith.ac.in/protien-misfolding-lab

PhD from : Banaras Hindu University, India

- Protein misfolding- mechanisms and prevention
- Yeast prions genetics and cell biology

Our laboratory investigates molecular mechanisms pertaining to misfolding of proteins and their consequent cytotoxicity. Another key focus of our laboratory is to find small molecule inhibitors to target protein misfolding towards therapeutic research.

In our laboratory, molecular mechanisms pertaining to misfolding of proteins and their consequent cytotoxicity is investigated. We use the yeast Saccharomyces cerevisiae model system and biochemical & biophysical tools for these studies. Another key focus of our laboratory is to find small molecule inhibitors to target protein misfolding towards therapeutic research. We also examine the role of chaperones and cellular pathways in mediating or mitigating the cytotoxicity due to protein misfolding and protein dyshomeostasis. We have carried out protein misfolding studies on TAR DNA binding protein 43 (TDP-43) implicated in the pathogenesis of amyotrophic lateral sclerosis (ALS) disease which is characterized by the loss of motor neurons that leads to the loss of movement, breathing and finally death of the patient. Our data suggests that Cyclin C, Dnm1 and Ybh3 proteins are important in mediating the TDP-43-induced oxidative stress-mediated cell death in the S. cerevisiae model. Also, using Alexa-fluor fluorescently labelled TDP-432C and TDP-432C-A315T proteins, we have shown that while these proteins manifest in vitro liquid-liquid phase separation (LLPS) giving spherical droplets, an additional presence of Zn2+ causes a solid-like phase separation. Also, recently we have shown that elevated constitutive expression of Hsp40 chaperone Sis1 reduces the TDP-43 aggregation-induced oxidative stress in the Ire1 pathway dependent-manner in the yeast TDP-43 proteinopathy model. Also, using in vitro studies we showed that a small organic molecule, AIM4, inhibits the aggregation and pathogenic LLPS of a familial ALS mutation (A315T)-bearing mutant C-terminal domain, TDP-432C-A315T.



PUBLICATIONS

Vidhya Bharathi, Amandeep Girdhar and Basant K Patel
Role of CNC1 gene in TDP-43 aggregation-induced oxidative stress-mediated cell death in S. cerevisiae model of ALS. 2021
BBA-Molecular Cell Research
doi: 10.1016/j.bbamcr.2021.118993.

Preethi S., Vidhya Bharathi and Basant K Patel.
Zn2+ modulates in vitro phase separation of TDP-432C and mutant TDP-432C-A315T C-terminal fragments of TDP-43 protein implicated in ALS and FTLD-TDP diseases. 2021
Int. J. Biol. Macromol.
DOI: 10.1016/j.ijbiomac.2021.02.054.

Amandeep Girdhar, Vidhya Bharathi, Tiwari, V.R., Abhishek, S., Deeksha, W., Mahawar, US., Raju, G., Singh, SK., Prabusankar, G., Rajakumara, E., and Basant K Patel
Computational insights into mechanism of AIM4-mediated inhibition of aggregation of TDP-43 protein implicated in ALS and evidence for in vitro inhibition of liquid-liquid phase separation (LLPS) of TDP-432C-A315T by AIM4. 2020
Int. J. Biol. Macromol.
DOI: 10.1016/j.ijbiomac.2020.01.032

Archana Prasad, Raju, G., Sivalingam, V., Girdhar, A., Verma, M., Vats, A., Taneja, V., Prabusankar, G., and Basant K Patel
An acridine derivative, [4,5-bis{(N-carboxy methyl imidazolium) methyl}acridine] dibromide, shows anti-TDP-43 aggregation effect in ALS disease models. 2016
Scientific Reports
doi: 10.1038/srep39490 (2016).

Archana Prasad, Vidhya Bharathi, Vishwanath, Sivalingam, Amandeep Girdhar and Basant K Patel.
Molecular Mechanisms of TDP-43 Misfolding and Pathology in Amyotrophic Lateral Sclerosis. 2019
Front Mol Neurosci.
https://doi.org/10.3389/fnmol.2019.00025.

COLLABORATIONS

Academic

1. Dr. G Prabushankar, IIT-Hyderabad, Hyderabad, India
2. Dr. Vibha Taneja, Sir Ganga Ram Hospital, New Delhi, India
3. Dr. Subhash C Yadav, AIIMS-New Delhi, India

AWARDS

1. Excellence in Teaching awards-2014, IIT-Hyderabad, India

Gaurav Sharma

Assistant Professor

Email: sharmaG@bt.iith.ac.in
Lab website: https://sites.google.com/view/sharmaglab/

PhD from CSIR-Institute of Microbial Technology, Chandigarh, India

- Microbial genomics and evolution
- Plant-microbe interactions
- Genomic, Metagenomic, and Transcriptomics
- Computational biology to function
- Next-generation sequencing data analysis
- Database and webserver development

My lab investigates high-throughput genome/ metagenome/transcriptome sequencing data, open-access omics data, and relevant metadata to enhance our understanding of microorganisms, their genetic diversity, peculiar pathways, evolutionary relationships, and ecological roles within diverse ecosystems.

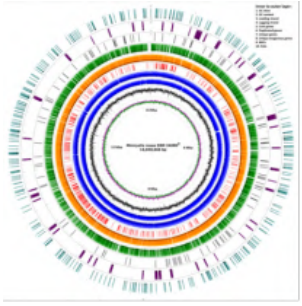
Our broad interest lies in exploring and understanding microbial diversity and genome evolution. With the development of remarkable sequencing technologies, an enormous amount of genome/ transcriptome/ metagenome data is being generated to infer interesting evolutionary theories, physiological behavior, and putative lifestyles of diverse organisms. We attempt to utilize this open-source data along with generating high throughput data from various sequencing platforms to bridge the gap between computational data, biological function, and organism evolution. A few significant directions are as follows:

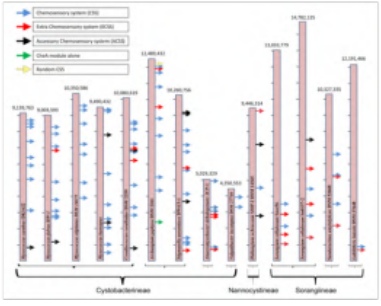
1) Understanding the genomic complexity in myxobacteria: Myxobacteria (Phylum Myxococcota) is a group of the largest genome size constituting microorganisms with diverse peculiar physiological characteristics. We are interested in understanding how these organisms gained this much genomic content, how these characteristics evolved, and how the signal transduction supports these unique functions.

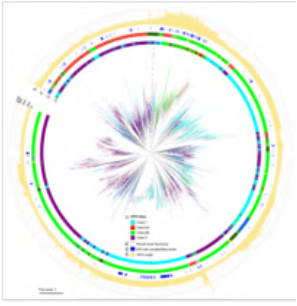
2) Diversity and evolution of microbes: My lab is also involved in understanding and exploring the distribution, function, and evolution of diverse pathways across available bacterial genomes in a high-throughput manner. Answering such talmudic questions allows us to get a bird's eye view of the Bacteria kingdom and its evolution.

3) Host-microbe interactions using computational microbiome studies: We use host genomics and community metagenomics to understand the medicinal plant-microbe interactions to comprehend the role of microbes in their secondary metabolite production.

4) Prediction webservers: We compile genomics/phylogeny-driven computational web-based tools to predict novel functions of proteins or their associated pathways that might help experimental biologists analyze and understand their input genomic and metagenomic sequences.







PUBLICATIONS

Richa Ashok Kakkar, Mariam Azeezuddin Haneen, Akash Chandra Parida, and Gaurav Sharma*
The Known, Unknown, and the Intriguing about members of a Critically Endangered Traditional Medicinal Plant Genus Aconitum
2023
Frontiers in Plant Sciences
https://www.frontiersin.org/articles/10.3389/fpls.2023.1139215/abstract

Kishan Kalia, Gayatri Saberwal, and Gaurav Sharma*
The lag in SARS-CoV-2 genome submissions to GISAID.
2021
Nature Biotechnology
https://www.nature.com/articles/s41587-021-01040-0

Fares Saïdi, Utkarsha Mahanta, Adyasha Panda, Nicolas Y. Jolivet, Razieh Bitazar, Gavin John, Matthew Martinez, Abdelkader Mellouk, Charles Calmettes, Yi-Wei Chang, Gaurav Sharma*, Salim T. Islam*
Bacterial Outer Membrane Polysaccharide Export (OPX) Proteins Occupy Three Structural Classes with Selective b-Barrel Porin Requirements for Polymer Secretion.
2022
Microbiology Spectrum
https://journals.asm.org/doi/10.1128/spectrum.01290-22

Gaurav Sharma, Andrew I. Yao, Gregory T. Smaldone, Jennifer Liang, Matt Long, Marc T. Facciotti, Mitchell Singer
Global gene expression analysis of the Myxococcus xanthus developmental time course.
2021
Genomics
https://www.sciencedirect.com/science/article/pii/S0888754320320346

Gaurav Sharma, Indu Khatri, Srikrishna Subramanian.
Comparative genomic analysis of diverse chemosensory systems in order Myxococcales
2017
Journal of Bacteriology
https://journals.asm.org/doi/10.1128/JB.00620-17

COLLABORATIONS

Academic

1. Prof. Salim Timo Islam, INRS, Canada
2. Prof. Mitchell Singer, University of California Davis, USA
3. Prof. Emina A. Stojković, Northeastern Illinois University, Chicago, USA
4. Dr. Qazi Parvaiz Hassan, CSIR-IIIM, Jammu and Kashmir, India
5. Dr. Rachna Chaba, IISER Mohali, India

AWARDS

1. Association of Microbiologists of India (AMI) Young Scientist Award (2022)
2. DST-INSPIRE Faculty Fellowship from DST India (2019)
3. European Molecular Biology Organization (EMBO) Travel Award (2019)
4. American Society for Microbiology Postdoctoral Travel Award (2018)
5. Editor at Microbiology Spectrum (ASM Publication) and Associate Editor for Genomics journal

Gunjan Mehta

Assistant Professor

Email: gunjanmehta@bt.iith.ac.in
Lab website: www.mehtalab-iith.com

PhD from Indian Institute of Technology Bombay, India

- Chromosome Dynamics and Cell Division
- Gene Regulation
- Aneuploidy, Genetic Disorders, Cancers
- Single-Molecule Imaging and Tracking

Understanding the molecular mechanism of chromosome segregation and gene regulation during mitosis and meiosis with cutting edge single-molecule imaging, cell and molecular biology, genomics/ transcriptomics, and yeast genetics.

Cell division and gene regulation are fundamental processes of life and they are tightly regulated for the precise execution of the cell survival, growth and reproduction. My lab aims to understand the molecular mechanism of cell division/chromosome segregation and gene regulation during mitosis and meiosis using cutting-edge single-molecule imaging, genomics, transcriptomics, cell and molecular biology and yeast genetics

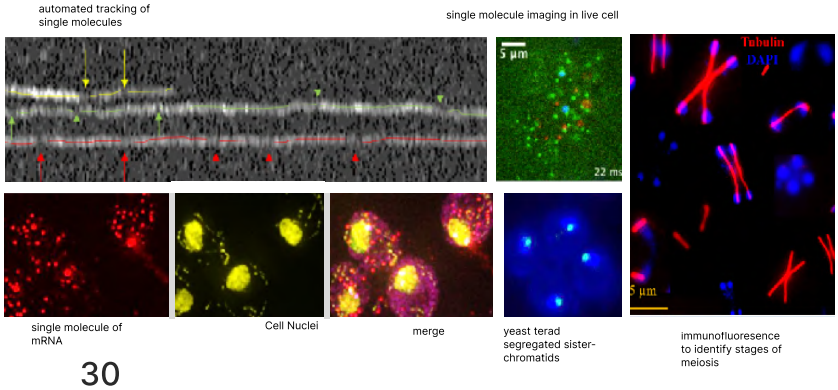
1) Unravelling the functions of ATP-dependent chromatin remodelers during meiosis, especially in meiotic recombination, chromosome segregation, and regulating the transcriptional switch of meiosis specific genes

2) Exploring the cohesin ring independent functions of cohesin subunits during meiotic chromosome segregation

3) Understanding the dynamic interplay between mitotic kinases (aurora kinases, polo kinase, cyclin-dependent kinases (Cdks), Mps1, Bub1) and phosphatases (protein phosphatase 1 (PP1), protein phosphatase 2A (PP2A)) during cell division using single-molecule imaging and tracking

4) Understanding the mechanism of epigenetic transcription memory/mitotic bookmarking using yeast as a model system

5) Exploring how the mitotic to meiotic transition is achieved at the level of 3D genome organization, kinetochore composition and transcriptome. We develop cutting-edge single-molecule imaging approaches, in collaboration with several national and international research groups, to understand these molecular mechanisms. Our basic science research efforts are geared towards developing therapeutics to treat infertility, genetic disorders and cancers.



PUBLICATIONS

Podh NK, Das A, Dey P, Paliwal S, Mehta G.
Single-Molecule Tracking for studying protein dynamics and target-search mechanism in live cells of S. cerevisiae.
2022
STAR Protocols (Cell Press)
https://doi.org/10.1016/j.xpro.2022.101900

Podh NK, Paliwal S, Dey P, Das A, Morjaria S, Mehta GD
In-vivo Single-Molecule Imaging in Yeast: Applications and Challenges.
2021
Journal of Molecular Biology
https://doi.org/10.1016/j.jmb.2021.1672503

Mehta GD, Ball DA, Eriksson PR, Chereji RV, Clark DJ, McNally JG, Karpova TS.
Single-Molecule analysis reveals linked cycles of RSC chromatin remodeling and Ace1 transcription factor binding in yeast.
2018
Molecular Cell
https://doi.org/10.1016/j.molcel.2018.09.009

Ball D, Mehta GD, Salomon-Kent R, Mazza D, Morisaki T, Mueller F, McNally JG, Karpova T.
Single-molecule tracking of Ace1p in Saccharomyces cerevisiae defines a characteristic residence time for non-specific interactions of transcription factors with chromatin.
2016
Nucleic Acids Research
https://doi.org/10.1093/nar/gkw744

Mehta GD, Agarwal M, Ghosh SK.
Functional characterization of kinetochore protein, Ctf19 in meiosis I: an implication of differential impact of Ctf19 on the assembly of mitotic and meiotic kinetochores in Saccharomyces cerevisiae.
2014
Molecular Microbiology
https://doi.org/10.1111/mmi.12527

COLLABORATIONS

Academic

1. Prof. Akira Shinohara, Osaka University, Japan
2. Prof. Tomoyuki Tanaka, University of Dundee, UK
3. Dr. Dimple Notani, NCBS, Bangalore, India
4. Dr. Shweta Tyagi, CDFD, Hyderabad, India
5. Dr. Saravanan Palani, IISc Bangalore, India

Industrial

1. Dr. Rashbehari Tunga, Ameliorate Biotech, Bangalore, India

AWARDS

1. JICA FRIENDSHIP2 Research Grant in collaboration with Osaka University, Japan (2023)
2. Ramalingaswami Fellowship from DBT, Govt. of India (2021)
3. Har-Govind Khorana Innovative Young Biotechnologist Award, DBT, Govt. of India (2020)
4. Fellows Award for Research Excellence (FARE), NIH, USA (2019)
5. Best Review Paper of the year 2014, IIT Bombay, India (2014)

Himanshu Joshi

Assistant Professor

Phone: 040 23016026
Email: hjoshi@bt.iith.ac.in
Lab website: sites.google.com/view/molecular-simulation-lab

PhD from IISc Bangalore 2017.

- DNA Nanotechnology
- Lipid-DNA, DNA-protein, and DNA-DNA interaction
- Artificial water channels
- Nanopores
- Nanoparticles and biological materials

Designing artificial water channels for water desalination, computationally assessing the ligand-protein binding. Characterizing the nanoscale structure, dynamics and thermodynamic properties of functional DNA nanostructure.

Richard Feynman once said, “everything that living things do can be understood in terms of the jigglings and wigglings of atoms.” Using computational methods, our group thrive to understand the bulk behaviour of the biological matter that emerges from the detailed structure and dynamics of molecules at the nanoscale. We use physics-based computational methods blended with statistical mechanics to understand and predict biological form and function. Our group excels in the all-atom and coarse-grained molecular dynamics simulation method and harnesses the power of high-performance supercomputers to create advances in the area of nanobiotechnology. The goal of our research group is to decipher the interaction that governs the behaviour of biomolecules and led up to what we call "Life". In this process of understanding the biomolecular form and function, we ask the question "can we create the synthetic analogue of the cellular components and use them to solve real-world problems like water desalination, drug design, nanomedicine etc.

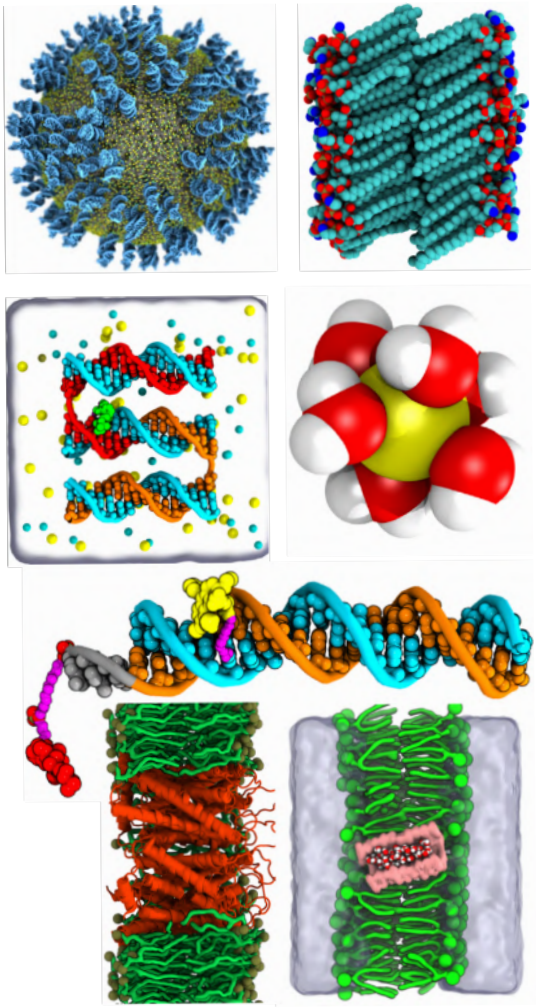


Figure: 1: Atomistic models of some of the nano-biosystems studied in our computational laboratory of nanobiotechnology.

PUBLICATIONS

- Himanshu Joshi, Atul Kaushik, Nadrian C Seeman, and Prabal K Maiti.
  Nanoscale structure and elasticity of pillared DNA nanotubes. **ACS NANO**, 10(8):7780-7791, 2016.
  https://pubs.acs.org/doi/abs/10.1021/acsnano.6b03360

- Dhiraj Bhatia, Senthil Arumugam, Michel Nasilowski, Himanshu Joshi, Christian Wunder, Val´erie Chambon, Ved Prakash, Chlo´e Grazon, Brice Nadal, Prabal K Maiti, Ludger Johannes, Benoit Dubertret, and Yamuna Krishnan. Quantum dot-loaded monofunctionalized DNA icosahedra for single-particle tracking of endocytic pathways. **Nature Nanotechnology**, 11(12):1112–1119, 2016.
  https://www.nature.com/articles/nnano.2016.150

- Arundhati Roy, Jie Shen, Himanshu Joshi, Woochul Song, Yu-Ming Tu, Ratul Chowdhury, Ruijuan Ye, Ning Li, Changliang Ren, Manish Kumar, Aleksei Aksimentiev, and Huaqiang Zeng.
  Foldamer-Based Ultrapermeable and Highly Selective Artificial Aquaporins that Exclude Protons. **Nature Nanotechnology**, 16, 911-917, 2021.
  https://www.nature.com/articles/s41565-021-00915-2

- Woochul Song, Himanshu Joshi, Ratul Chowdhury, Joseph S. Najem, Yue xiao Shen, Chao Lang, Codey B. Henderson, Yu-Ming Tu, Megan Farell, Megan E. Pitz, Costas D. Maranas, Paul S. Cremer, Robert J. Hickey, Stephen A. Sarles, Jun li Hou, Aleksei Aksimentiev, and Manish Kumar.
  Artificial water channels enable fast and selective water permeation through water-wire networks. **Nature Nanotechnology**, 15:73–79, 2020.
  https://www.nature.com/articles/s41565-019-0586-8

- Himanshu Joshi and Prabal K Maiti.
  Structure and electrical properties of DNA nanotubes embedded in lipid bilayer membranes. **Nucleic Acids Research**, 46(5):2234-2242, 11, 2017.
  https://academic.oup.com/nar/article-abstract/46/5/2234/4612966

COLLABORATIONS

Academic

1. Huaqiang Zeng, Fuzhou University, China
2. Manish Kumar, University of Texas at Austin , USA
3. Aleksei Aksimentiev, University of Illinois at Urbana-Champaign, USA
4. Mukund Ramakrishnan, IISER Berhampur, India
5. Ravindra Kumar Pandey IIT Roorkee, India

AWARDS

1. SHELL India Computational Talent Prize, 2016,
2. DST Inspire Faculty Fellowship, 2021.
3. Start-Up Research Grant, SERB 2022

PATENTS

1. High-Affinity Oligonucleotide Nanomatrix and Nanocarrier system. Submitted, Indian Patent Application no. 202341006125

Indranil Malik

Assistant Professor

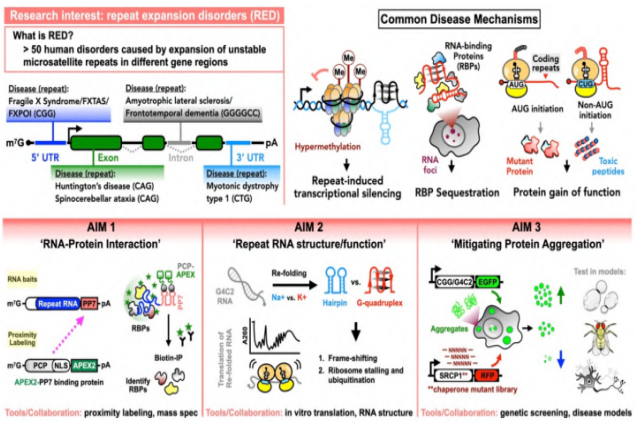
Email: indranil@bt.iit.ac.in
Lab website:https://sites.google.com/bt.iith.ac.in/malik-lab/home

PhD from Texas A&M University – College Station, Texas, USA

- Repeat Expansion Disorders
- Role of RNA binding proteins in neurological diseases
- RNA structure and translational regulation
- Developing Drosophila models of human neurodegenerative diseases

We are using a multi-pronged approach to study RNA metabolism dysfunction in health and diseases, with the goal of developing RNA-targeting therapeutics.

Our long-term goal is to study fundamental mechanisms of gene expression process in relation to human diseases and utilize this work to develop novel therapeutic strategies. In our lab, we are adapting novel tools to study the roles of repeat RNA-associated toxicity in a group of neurodegenerative disorders commonly known as 'Repeat expansion disorders'. We seek to identify novel RNA-binding proteins (RBPs) that interact with expanded repeat RNAs, determine the in vivo structures of different RNA repeats, and then combine these two datasets to determine how specific RBPs facilitate the translation of these disease-causing 'toxic' RNAs. Additionally, we want to understand how alterations in fundamental aspects of RNA homeostasis may contribute to human diseases, which include but are not limited to neurodegenerative disorders. Our current research is focused on the following areas – I. Develop/utilize cutting-edge techniques to detect RNA-protein interactions. Define the subcellular and context-specific repeat RNA-protein interactome. Characterize the roles of disease associated RBPs in fly and neuronal models of repeat expansion disorders; II. Develop/utilize chemical, mutational, and sequencing-based techniques for the analysis of multiple disease-associated repeat RNA structures. Determine how RNA structure/folding may contribute to translational regulations. Use the RNA structural information to develop/screen for chemical inhibitors of repeat-RNA associated toxicity; III. We are also interested in employing novel molecular chaperones (such as serine-rich chaperone protein 1 or, SRCP1 from Dictyostelium discoideum) to directly counter toxic aggregation-prone repeat peptides produced through translation of repeat RNAs.



PUBLICATIONS

Malik I, Tseng YJ, Wieland CM, Green KM, Zheng K, Calleja K, Todd PK.
Dissecting the roles of EIF4G homologs reveals DAP5 as a modifier of CGG repeat-associated toxicity in a Drosophila model of FXTAS.
2023
Neurobiol Dis.
doi: 10.1016/j.nbd.2023.106212.

Malik I, Tseng YJ, Wright SE, Zheng K, Ramaiyer P, Green KM, Todd PK.
SRSF protein kinase 1 modulates RAN translation and suppresses CGG repeat toxicity.
2021
EMBO Mol Med.
doi: 10.15252/emmm.202114163.

Malik I*, Kelley CP*, Wang ET, Todd PK.
Molecular mechanisms underlying nucleotide repeat expansion disorders.
2021
Nat Rev Mol Cell Biol.
doi: 10.1038/s41580-021-00382-6.

Malik I, Qiu C, Snavely T, Kaplan CD.
Wide-ranging and unexpected consequences of altered Pol II catalytic activity in vivo.
2017
Nucleic Acids Res.
doi: 10.1093/nar/gkx037.

Barnes CO*, Calero M*, Malik I, Graham BW, Spahr H, Lin G, Cohen AE, Brown IS, Zhang Q, Pullara F, Trakselis MA, Kaplan CD, Calero G.
Crystal Structure of a Transcribing RNA Polymerase II Complex Reveals a Complete Transcription Bubble.
2015
Mol Cell.
doi: 10.1016/j.molcel.2015.06.034.

COLLABORATIONS

Academic

1. Dr. Silvi Rouskin, Harvard University, USA
2. Dr. Peter K. Todd, University of Michigan, USA
3. Dr. James Bardwell, University of Michigan, USA

AWARDS

1. Alzheimer's Association Research Fellowship (AARF-20-684648), 2020-23.
2. RNA Society 'poster recognition award' sponsored by National Science Foundation (NSF), USA. 2021
3. College of Agriculture and Life Sciences 'Excellence Fellowship', Texas A & M University – College Station, Texas, USA. 2011-12

N K Raghavendra

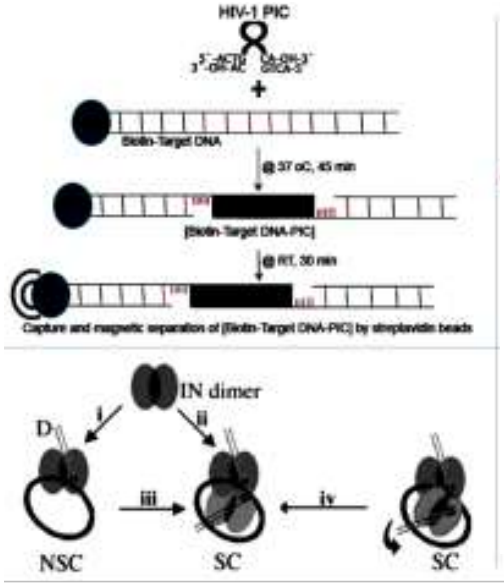
Associate Professor

Email: raghunk@bt.iith.ac.in
Lab website: https://sites.google.com/iith.ac.in/pial/home

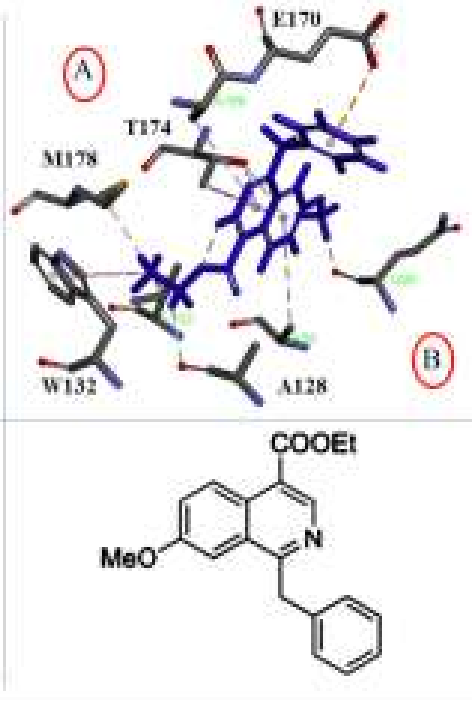
PhD from Indian Institute of Science Bangalore, India.

Human – virus: protein-protein and DNA-protein interaction

Broadly, understanding how the interaction of viral proteins, in the cytoplasm of a susceptible cell, with the host proteins, alters the functionality of both the interacting partners, forms the core of research. Towards this, techniques involving molecular biology, biochemistry, ectopic expression of proteins in mammalian cell culture and pseudovirus infection of cell lines, are employed.



The focus of research in the laboratory is primarily on proteins of two viruses that infect humans. First, is the interaction of HIV-1 enzyme integrase with the cytoplasmic proteins of the susceptible cells. Second, is that of SARS-CoV-2 structural protein Spike with ACE-2 and TMPRSS-2 of susceptible cells. Site-directed mutagenesis of virus and human protein partners are used to understand the chemistry at the protein-protein interface. The knowledge obtained from such studies is extended to design small molecule inhibitors of the interaction. Apart from studying the interactions using recombinant proteins, pseudovirus having the mutant form of the proteins are used to analyse the effects of mutations on the levels of infection in the susceptible mammalian cell lines. Docking software is employed to assist the design of mutants, as well as, to interpret the observations of the in vitro experiments.



PUBLICATIONS

MLY Bangaru, RK Medabalimi, S Babu, NK Raghavendra.
REMP software to introduce a screening REstriction site in site-directed Mutagenesis Primer
2021
SoftwareX
https://doi.org/10.1016/j.softx.2021.100881

A George, A Gopi Krishna Reddy, G Satyanarayana, NK Raghavendra.
1, 2, 3, 4-Tetrahydroisoquinolines as inhibitors of HIV-1 integrase and human LEDGF/p75 interaction
2018
Chemical Biology & Drug Design
https://doi.org/10.1111/cbdd.13175

A George & NK Raghavendra.
L368F/V408F double mutant of IBD of LEDGF/p75 retains interaction with M178I mutant of HIV-1 integrase
2017
Biochemical and biophysical research communications
https://doi.org/10.1016/j.bbrc.2017.06.035

NK Raghavendra, N Shkriabai, RLJ Graham, S Hess, M Kvaratskhelia & L Wu.
Identification of host proteins associated with HIV-1 preintegration complexes isolated from infected CD4+ cells
2010
Retrovirology
https://doi.org/10.1186/1742-4690-7-66

MC Shun, NK Raghavendra, N Vandegraaff, JE Daigle, Hughes S, Kellam P, Cherepanov P, Engelman A.
LEDGF/p75 functions downstream from preintegration complex formation to effect gene-specific HIV-1 integration
2007
Genes & Development
http://www.genesdev.org/cgi/doi/10.1101/gad.1565107

COLLABORATIONS

Academic

1. Prof. Raghavan Varadarajan, MBU, IISc Bangalore.
2. Prof. Ranga Udaykumar, MBGU, JNCASR, Bangalore.
3. Prof. G. Satyanarayana, Chemistry, IIT Hyderabad.
4. Prof. Sobhan Babu, CSE, IIT Hyderabad.

AWARDS

1. Member, BoS, Biotechnology, K.L.E. Technological University, Hubli. KA. (2022-present)
2. External member, IBSC, University of Hyderabad (2020-2023).
3. Illustrious alumnus at Silver Jubilee celebrations of St. Joseph's Degree College, Kurnool. AP. (2020).
4. Invited Speaker at International Conference on Biology And Therapeutics of HIV & Associated Infections, University of Hyderabad. (2018)
5. Invited Speaker at TRendys in Biochemistry, Ancharya Nagarjuna Univeristy, AP (2014)
6. Invited Speaker at NanoTech Conference, Ancharya Nagarjuna Univeristy, AP (2012)
7. 'Excellence in Teaching' award by IIT Hyderabad (academic year 2012-13)

Rahul Kumar

Assistant Professor

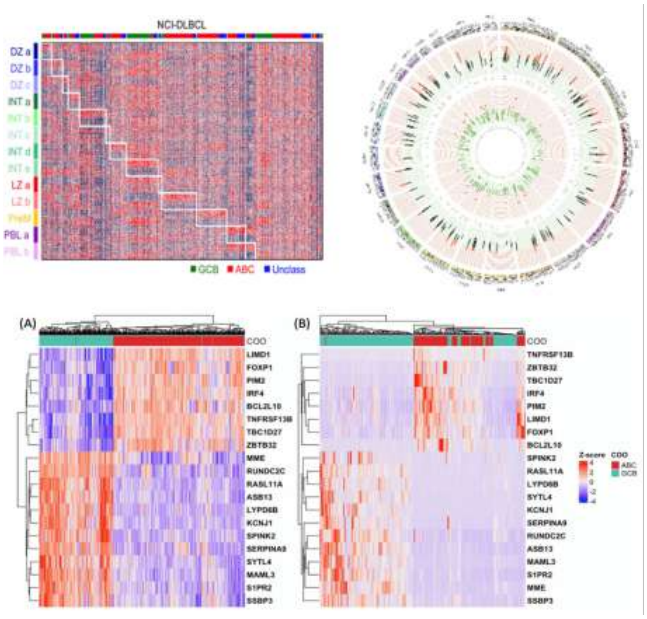
Email: rahulk@bt.iith.ac.in
Lab website: https://sites.google.com/view/rahulklab/

PhD from CSIR-Institute of Microbial Technology, Chandigarh, India

- Radiogenomics based biomarkers for glioblastoma prognosis and diagnosis
- Developing AI/ML based methods to design novel anticancer compounds
- Developing multi-omics biological databases
- Developing AI/ML based algorithms to identify novel molecular subtypes
- Exploring non-coding elements for disease pathology

Deploying computational tools on high throughput multi-omics data to delineate the novel mechanism of cancer progression. Utilising power of AI/ML techniques to develop predictive biomarkers of survival outcomes of cancer patients.

Advancement in sequencing technologies lead to the generation of high volume (big data) of multi-omics data for almost all the cancer types. This big multi-omics data of thousands of cancer patients provides an unique opportunity to understand the disease pathophysiology and design new therapies. Recently, our research group developed a deep-learning based classification method to stratify diffuse large B-cell lymphoma (DLBCL) patients into ABC and GCB subtypes using transcriptomics data. We have also developed two multi-omics database for acute myeloid leukemia (AML) and multiple myeloma (ML) and identified novel biomarkers of these two cancer types. Along with multi-omics data, there is a surge in drug screening data which we utilised to develop AI/ML based quantitative structure activity relationship (QSAR) models to design effective molecules against colorectal cancer. Non-invasive method of cancer detection is always an important aspect and in that direction MR imaging of brain play a critical role to detect glioblastoma. We are leveraging the power of both radiomics (MRI based approach) and genomics to design novel prognostic biomarkers for glioblastoma



PUBLICATIONS

Viswanathan A, Kundal K, Sengupta A, Kumar A, Kumar K V, Holmes A B, Kumar R
Deep learning-based classifier of diffuse large B-cell lymphoma cell-of-origin with clinical outcome
2023
Briefings in Functional Genomics
https://academic.oup.com/bfg/article/22/1/42/6835328

Elodie Bal, Rahul Kumar, Mohammad Hadigol, Antony B Holmes, Laura K Hilton, Jui Wan Loh, Kostiantyn Dreval, Jasper CH Wong, Sofija Vlasevska, Clarissa Corinaldesi, Rajesh Kumar Soni, Katia Basso, Ryan D Morin, Hossein Khiabanian, Laura Pasqualucci, Riccardo Dalla-Favera
Super-enhancer hypermutation alters oncogene expression in B cell lymphoma
2022
Nature
https://www.nature.com/articles/s41586-022-04906-8

Ambuj Kumar, Keerthana Vinod Kumar, Kavita Kundal, Avik Sengupta, Kunjulakshmi R, Rahul Kumar
MyeloDB: A multi-omics resource for Multiple Myeloma.
2023
bioRxiv
https://www.biorxiv.org/content/10.1101/2023.05.18.541396v1

Keerthana Vinod Kumar, Ambuj Kumar, Kavita Kundal, Avik Sengupta, Kunjulakshmi R, Mayilaadumveettil Nishana, Rahul Kumar
AMLdb: A comprehensive multi-omics platform to understand the pathogenesis and discover biomarkers for acute myeloid leukemia.
2023
bioRxiv
https://www.biorxiv.org/content/10.1101/2023.05.19.541403v1

Ambuj Kumar, Keerthana Vinod Kumar, Kunjulakshmi R, Kavita Kundal, Avik Sengupta, Rahul Kumar
Advancement of in silico tools for stem cell research
2023
Book chapter in Computational Biology for Stem Cell Research
Accepted

COLLABORATIONS

Academic

1. Dr. Shantanu Chowdhury, Chief Scientist, CSIR-IGIB
2. Dr. Saran Kumar, Assistant Professor, IIT Delhi
3. Dr. Nishana, Assistant Professor, IISER TVM
4. Dr. Sushil Kumar, Assistant Profeeosr, IIT Bombay
5. Dr. Bhawana Tiwari, DBT-Wellcome Fellow, IISER Behrampur

AWARDS

1. Best PhD Thesis award
2. Committee member in Telangana State Council of Higher Education (TSCHE) for designing Bioinformatics curriculum at UG & PG level in Telangana state colleges.
3. Selected as one of the best performers in Network Verification Challenge (NVC) conducted by Philip Morris International (PMI) and IBM all over the world in 2014.

Rajakumara Eerappa

Associate Professor

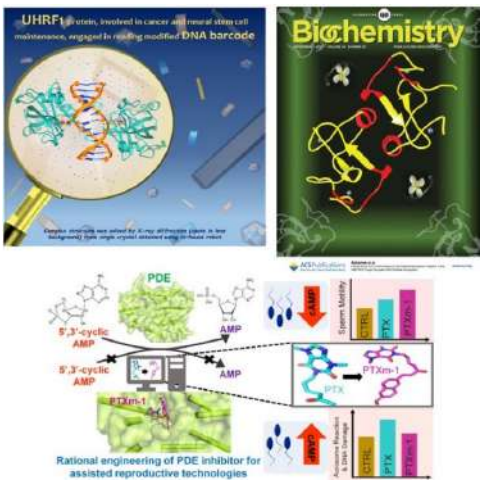
Email: eraj@bt.iith.ac.in
Lab website: https://www.rajlab-bt-iith.com/

PhD from CSIR-The Centre for Cellular & Molecular Biology, India

- Epigenetics, DNA repair and allosteric regulation of receptors and enzymes
- Characterization of cancer drug targets, Inhibitor/lead compound design
- Thermodynamics of phase separation of biological macromolecules and hydrogel design
- X-ray crystallography and Structural Biology

Using complementary approaches (structural, computational, biochemical & biophysical) that each feed into one another, we investigate the macromolecular-mediated recognition, validation of drug targets, catalysis & enzyme engineering, and inhibitors/drug/ vaccine design.

Poly (ADP-ribose) polymerase (PARP) 1 and 2 are referred to as “genome guardians”, as they play a very crucial role in maintaining the genome integrity. PARP inhibitors (PARP(i)) are approved for the treatment of multiple cancers. We unravel the mechanism of allosteric regulation of DNA breaks recognition and catalytic activities of PARP1 and 2 by their catalytic product poly ADP ribose (PAR) polymer, RNA and PARP(i)s. The outcome of this work would lead to the development of PARP-specific inhibitor drugs for different cancers treatment. We also design phosphodiesterase inhibitors to modulate sperm functions, such as sperm motility, longevity, and pre-acrosomal reactions, for assisted reproductive technologies including IVF and intracytoplasmic sperm injection. We also investigate the epigenetic marks such as histone methyl-lysine and CpG methylation recognition by the reader domains of different modular proteins such as UHRF1, SUVH5, and ATP-dependent chromatin remodelers such as CHD1. Further, we characterize the topological modulation of mitochondrial DNA of the human pathogen Trypanosoma by HMGB proteins. We also investigate the thermodynamics of macromolecules, such as poly ADP ribosylated (PARylated) proteins and DNA, phase separation, and the use of PARylated proteins and PAR to design hydrogels and layer-by-layer assemblies for biomedical applications. My lab also aims to characterize and/or engineer enzymes for chiral APIs and fine chemical synthesis.



PUBLICATIONS

Deeksha W, Abhishek S, Giri J, Rajakumara E
Regulation of PARP1 and its apoptotic variant activity by single-stranded DNA
2023
FEBS J
Accepted

Abhishek S, Deeksha W, Rajakumara E
Mechanistic insights into allosteric regulation of methylated DNA and histone H3 recognition by SRA and SET domains of SUVH5 and the basis for di-methylation of lysine residue
2023
FEBS J
doi: 10.1111/febs.16633.

Pratibha M, Abhishek S, Rajakumara E
Designing ferritin nanocage based vaccine candidates for SARS-CoV-2 by in silico engineering of its MHC I and MHC II epitope peptides.
2022
J Biomol Struct Dyn
doi: 10.1080/07391102.2022.2103027

Satish M, Kumari S, Deeksha W, Abhishek S, Nitin K, Adiga SK, Hegde P, Dasappa JP, Kalthur G, Rajakumara E.
Structure-based redesigning of pentoxifylline analogs against selective phosphodiesterases to modulate sperm functional competence for assisted reproductive technologies,
2021
Nature Scientific Reports
doi: 10.1038/s41598-021-91636-y
https://youtu.be/grUr-9_X7cw.

Abhishek S, Nakarakanti NK, Deeksha W, Rajakumara E
Mechanistic insights into recognition of symmetric methylated cytosines in CpG and non-CpG DNA by UHRF1 SRA.
2021
Int J Biol Macromol.
doi: 10.1016/j.ijbiomac.2020.12.149

COLLABORATIONS

Academic

1. Porf. Guruprasad Kalthur, Department of Clinical Embryology, Kasturba Medical College, Manipal Academy of Higher Education
2. Dr. Mehdi D. Davari, Research group leader in Computational Chemistry at Leibniz Institute of Plant Biochemistry (IPB), Weinberg, Germany
3. Dr. Simon Moulton, Professor of Biomedical Electromaterials Science, Iverson Health Innovation Research Institute, Swinburne University of Technology, Australia
4. Prof. Sumohana Channappayya, Electrical Engineering Department, IIT Hyderabad
5. Dr. Priyanka Bajaj, Assistant Professor, Department of Pharmaceutical Technology NIPER Hyderabad

Industrial

1. Boltzmann company (https://boltzmann.co/), Bengaluru, India

AWARDS

1. DAAD Scholarship, Research Stays for University Academics and Scientists, German Academic Exchange Service (2019).
2. Guest Professor in Prof. Dr. Ulrich Schwaneberg Group, Chair of Biotechnology, ABBt Institute of Biotechnology, RWTH Aachen University, Germany (2019.
3. Early Career Research Award, Science & Engineering Research Board (SERB), Department of Science & Technology (DST) (2016).
4. Ramalingaswami Re-entry fellowship, Department of Biotechnology (DBT), Government of India (2014).
5. Structured International Postdoc Program (SIPAD) fellowship sponsored by European School of Molecular Medicine and, co-funded by European Commission in the context of 'FP7 program Marie Curie Actions- people'

PATENTS

1. 202341028077
   Enzymatic synthesis of a novel anionic polymer: Poly(Cytidine diphosphate ribose)
   Dr. Rajakumara Eerappa, Ms. Deeksha Waghela
2. 202341028076
   Synthesis and evaluation of inhibitor against phosphodiesterases PDE4A, PDE4D, and PDE10
   Dr. Rajakumara Eerappa, Prof. G. Satyanarayana, Mr. Raj Virendra Gupta, Mr. M. Ramachandra Reddy

Sandipan Ray

Assistant Professor

Email: sandipan.ray@bt.iith.ac.in
Lab website: www.circadianlab-iith.com

Ph.D. from Indian Institute of Technology Bombay, India

- Circadian rhythms and sleep
- Neuropharmacology
- Aging
- Mental health
- Systems biology

We are investigating circadian clock-oriented therapeutics for chronic human diseases such as mental disorders, cardiovascular diseases, and cancers. We are conducting systems-level studies to integrate physiological underpinnings among circadian rhythms, sleep, mental health, and aging.

Circadian Involvements in Mental Health
Mental illnesses are one of the significant causes of disease burden. In this project, we intend to compare the circadian amplitude parameter in bipolar disorder (BD) patients measured by actigraphy and by rhythmic expression or abundance of core clock genes and metabolites. We also intend to understand the circadian control of pathogenic disease factors and therapeutic drug targets.

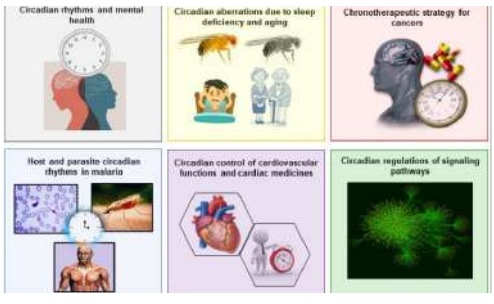
Cross-talk among Circadian Disruption, Sleep Deficiency, and Aging:
Aging and sleep deficiency are variables that can perturb circadian clock regulation and potentially increase the risk for diverse chronic diseases. We aim to decode healthy aging by providing accurate circadian measures or predictors through cutting-edge omics-based high throughput technologies.

Dosing Time Dependency of Anticancer Drugs:
In this project, we investigate the dosing time dependency of anticancer drugs (breast cancer, colorectal cancer, and retinoblastoma) and their metabolic pathways. We are also interested in understanding the molecular mechanisms and cellular responses of novel pharmacological modulators of the mammalian circadian clock with potential anticancer properties.

Host and Parasite Rhythms in Malaria:
In this project, we systematically investigate the circadian proteome and metabolome of the in-vitro cultured Plasmodium falciparum strains and falciparum malaria patients' serum and RBC using mass spectrometry-based approaches.

Circadian Regulations of Kinases and Diverse Signaling Pathways:
Circadian regulation of kinases and signaling pathways is mostly undefined. This project uses an integrated quantitative proteomics pipeline to investigate the circadian regulations in the expression and activity profiles of kinases and their associated signaling pathways.

Circadian Disruptions in Cardiovascular Diseases:
Coronary artery diseases such as myocardial infarction can be correlated with the consequences of circadian time-keeping system dysfunction. In this project, our research strategy focuses on unraveling circadian regulation and anomalies in young and elderly cardiovascular disease patients and circadian regulation of cardiac medicine.



PUBLICATIONS

Banerjee S, Ray S
Circadian medicine for aging attenuation and sleep disorders: Prospects and challenges
2023 Progress in Neurobiology
https://www.sciencedirect.com/science/article/abs/pii/S0301008222001733?via%3Dihub

Ch R, Rey G, Ray S, Jha P, et al.
Rhythmic glucose metabolism regulates the redox circadian clockwork in human red blood cells
2021 **Nature Communications**
https://www.nature.com/articles/s41467-020-20479-4

Ray S, Valekunja UK, Stangherlin A, Howell SA, et al.
Circadian rhythms in the absence of the clock gene Bmal1
2020 **Science**
https://www.science.org/doi/10.1126/science.aaw7365?url_ver=Z39.88-2003&rfr_id=ori:rid:crossref.org&rfr_dat=cr_pub%20%200pubmed

Ray S, Lach R, Heesom KJ, Valekunja UK, et al.
Phenotypic proteomic profiling identifies a landscape of targets for circadian clock-modulating compounds
2019 **Life Science Alliance**
https://www.life-science-alliance.org/content/2/6/e201900603/tab-rc

Ray S, Reddy AB
COVID-19 management in light of the circadian clock
2020 **Nature Reviews Molecular Cell Biology**
https://www.nature.com/articles/s41580-020-0275-3y

COLLABORATIONS

Academic

1. Prof. Greg Murray, Swinburne University of Technology, Melbourne, Australia
2. Prof. Arunansu Talukdar, Medical College Kolkata, West Bengal, India
3. Dr. Aravind K. Rengan, Indian Institute of Technology Hyderabad, India
4. Prof. G. Narahari Sastry, CSIR North East Institute of Science and Technology, Jorhat, Assam, India
5. Prof. Richard Porter, University of Otago, Christchurch, New Zealand

Industrial

1. Dr. Durairaj Renu, Strand Life Sciences, Bangalore

AWARDS

1. 2023: Elected as an Executive Committee member of the Indian Society for Chronobiology (InSC)
2. 2021: Selected for Affiliate Membership of the Institute for Translational Medicine and Therapeutics, USA
3. 2020: Elected to the Royal Society of Biology, UK
4. 2018: Thermo Scientific Annual Tandem Mass Tag Research Award (International)
5. 2015: Excellence in Ph.D. Research Award 2014-2015 - IIT Bombay, Mumbai, India

PATENTS

1. Prof. Sanjeeva Srivastava, Dr. Sandipan Ray, Dr. Veenita Grover Shah. Label-Free Method for Detection and Quantification of Protein Biomarkers [India-Patent No. 394414 (Granted, Award Date: 07/04/2022)].
2. Prof. Sanjeeva Srivastava, Prof. Swati Patankar, Dr. Sandipan Ray, Dr. Urmila Thatte, Dr. Nithya Gogtay, Dr. Durairaj Renu, et al. Protein Biomarkers for Plasmodium vivax Malaria [India-Patent No. 336131 (Granted, Award Date: 28/04/2020)].
3. Prof. Sanjeeva Srivastava, Prof. Rajneesh Srivastava, Dr. Sandipan Ray, Mr. Vineet Vaibhav. Protein Biomarkers for Leptospirosis [India-Patent No. 336123 (Granted, Award Date: 28/04/2020)].
4. Prof. Sanjeeva Srivastava, Prof. Swati Patankar, Dr. Sandipan Ray, Dr. Urmila Thatte, Dr. Nithya Gogtay, Dr. Durairaj Renu, et al. Protein Biomarkers for Plasmodium falciparum Malaria [IPA No. 201922050215; Publication Date: 05/12/2019].
5. Prof. Sanjeeva Srivastava, Dr. Sandipan Ray, Mr. Vipin Kumar. Method for Detection of Protein Biomarkers for Different Complications of Falciparum Malaria [IPA No. 202021002027; Publication Date: 23/07/2021].

Thenmalarchelvi Rathinavelan

Associate Professor

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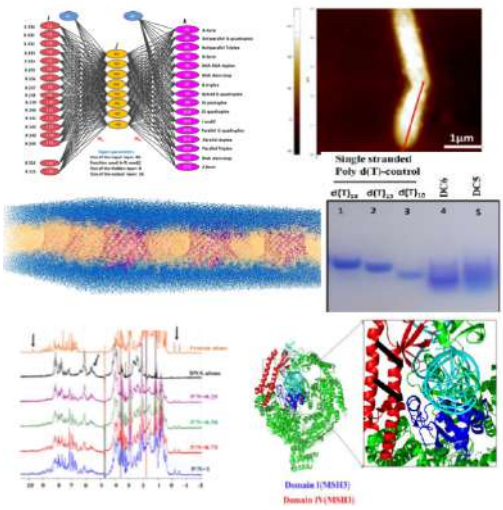
Email: tr@bt.iith.ac.in
Lab website: https://people.iith.ac.in/tr/Home.html

PhD from (Department of Crystallography & Biophysics, University of Madras)

- Molecular mechanism behind microsatellite repeat expansion disorders
- Antimicrobial resistance in Gram-negative bacteria
- Microbial genomics
- Amyloidogenic characteristic of an intrinsically disordered Saccharomyces cerevisiae protein
- Development of algorithms, databases and web tools
- Utilization of SERBP1 as an anticancer drug target
- Identification of ligand molecules to target microsatellite repeat expansions
- Biomolecular structure and interaction prediction using machine learning algorithms

To understand the physical principles behind the biological phenomena by employing computational, biophysical, biochemical and structural techniques.

Molecular biophysics lab explores the biological mechanisms in the perspective of human diseases and disorders by employing computational and experimental techniques. We are involved in the development of sophisticated databases and algorithms to store and analyze multiomics biological data to derive the hidden biological information. Development of web tools to i) predict proteome wide zinc finger domains/ motifs, (i) track the evolutionary dynamics of SARS-CoV-2, (iii) predict the secondary structure of the nucleic acids from circular dichroism spectra using machine learning algorithms, (iv) predict the serovars of Klebsiella, Acinetobacter and Salmonella and (v) automatically model nucleic acids secondary structures and, a repository of (vi) K-antigen E coli structures are the examples in this line. We also employ molecular dynamics simulation technique to understand the influence of base pair mismatches on the nucleic acids conformation and the concomitant impact on interaction with mismatch repair proteins and, conformational dynamics of bacterial membrane proteins in the perspective of microsatellite repeat expansion disorders and antimicrobial resistance respectively. Besides, we employ CD, microscale thermophoresis, EMSA, NMR and AFM techniques to explore the conformational dynamics of biomacromolecules and, to identify the influence of ligand molecules on the nucleic acids secondary structures and biomolecular interactions.



PUBLICATIONS

Chakkarai Sathyaseelan, L Ponoop Prasad Patro, Thenmalarchelvi Rathinavelan
Sequence patterns and HMM profiles to predict proteome wide zinc finger motifs
2023
Pattern Recognition
https://doi.org/10.1016/j.patcog.2022.109134

Patil Pranita Uttamrao, Chakkarai Sathyaseelan, L. Ponoop Prasad Patro, Thenmalarchelvi Rathinavelan
Revelation of Potent Epitopes Present in Unannotated ORF Antigens of SARS-CoV-2 for Epitope- Based Polyvalent Vaccine Design Using Immunoinformatics Approach
2021
Frontiers in Immunology
https://doi.org/10.3389/fimmu.2021.692937

Super-enhancer hypermutation alters oncogene expression in B cell lymphoma

2022 **Nature**
https://www.nature.com/articles/s41586-022-04906-8

Yogeeshwar Ajjugal, Y., Narendar Kolimi, N. Thenmalarchelvi Rathinavelan
Secondary structural choice of DNA and RNA associated with CGG/CCG trinucleotide repeat expansion rationalizes the RNA misprocessing in FXTAS
2021
Scientific reports
https://doi.org/10.1038/s41598-021-87097-y

Bharathi Reddy Kunduru, Sanjana Anilkumar Nair, Thenmalarchelvi Rathinavelan
EK3D: an E. coli K antigen 3-dimensional structure database
2016
Nucleic Acids Research
https://doi.org/10.1093/nar/gkv1313

Thenmalarchelvi Rathinavelan, Lara-Tejero, M., Lefebre, M., Chatterjee, S., McShan, A.C., Guo, D-C., Tang, C., Galan, J.E. and De Guzman, R.N.
NMR Model of PrgI–SipD Interaction and Its Implications in the Needle-Tip Assembly of the Salmonella Type III Secretion System
2014
Journal of molecular biology
https://doi.org/10.1016/j.jmb.2014.06.009

COLLABORATIONS

Academic

1. Prof Prabu Shankar, Department of Chemistry IITH, Hyderabad
2. Dr D. Fernando Estrada, University at Buffalo, USA
3. Dr Umakanta Subudhi, CSIR-Institute of Minerals and Materials Technology (IMMT), India
4. Dr Umashankar Singh, IIT Gandhinagar, India
5. Dr Krishna Rao, TCIS, Hyderabad

AWARDS

1. Innovative Young Biotechnologist Award 2012, DBT-Government of India, 2013
2. Excellence in Teaching Award 2014-2015, IIT Hyderabad, 2015
3. BIRAC-SRISTI-GYTI-Award, Honeybee Network-Department of Biotechnology, 2019
4. BIRAC-SRISTI-GYTI-Appreciation, Honeybee Network-Department of Biotechnology, 2018
5. BIRAC-SRISTI-GYTI-Award, Honeybee Network-Department of Biotechnology, 2017

Undurti N Das

Adjunct Professor

MD, DSc, FAMS, FRSC

Consultant Physician, Diabetologist, Clinical Immunologist, Rheumatologist, CEO, CSO, UND Life Sciences

2221 NW 5th St, Battle Ground, WA 98604, USA

- Area of Research: polyunsaturated fatty acids and their metabolism

Dr. G. Narahari Sastry

Adjunct Professor

FNA, FNASc, FASc, FRSC

Director CSIR-North East Institute of Science and Technology

Pulibor, Jorhat, Pin-785006 ,India

- computational modelling and artificial intelligence from basic to translational research

Dr. Neeraj Kumar

Affiliated Faculty

Assistant Professor, Liberal Arts. IIT Hyderabad

Room: C-112/F, Academic Block C Indian Institute of Technology Hyderabad Kandi-502284, Sangareddy Telangana, India

- Sensorimotor Learning, Motor Memory, Non-invasive Brain Stimulation, Stroke Rehabilitation.

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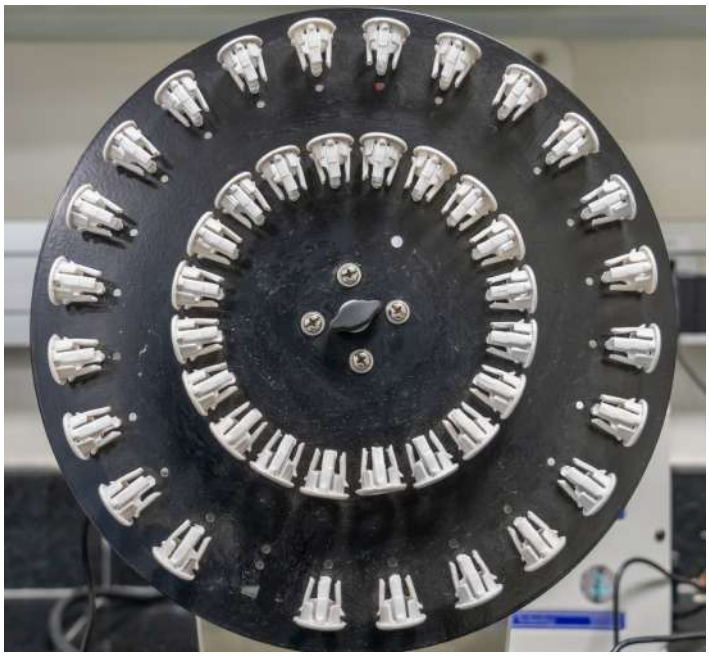
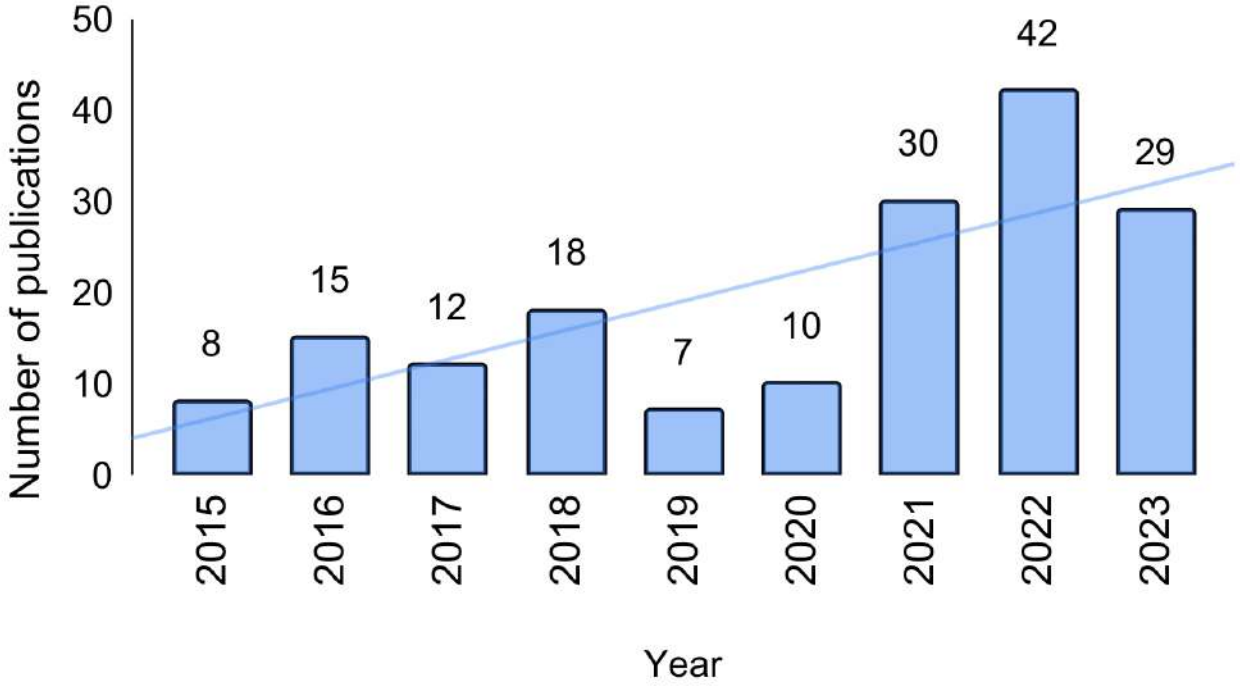
Research Facilities

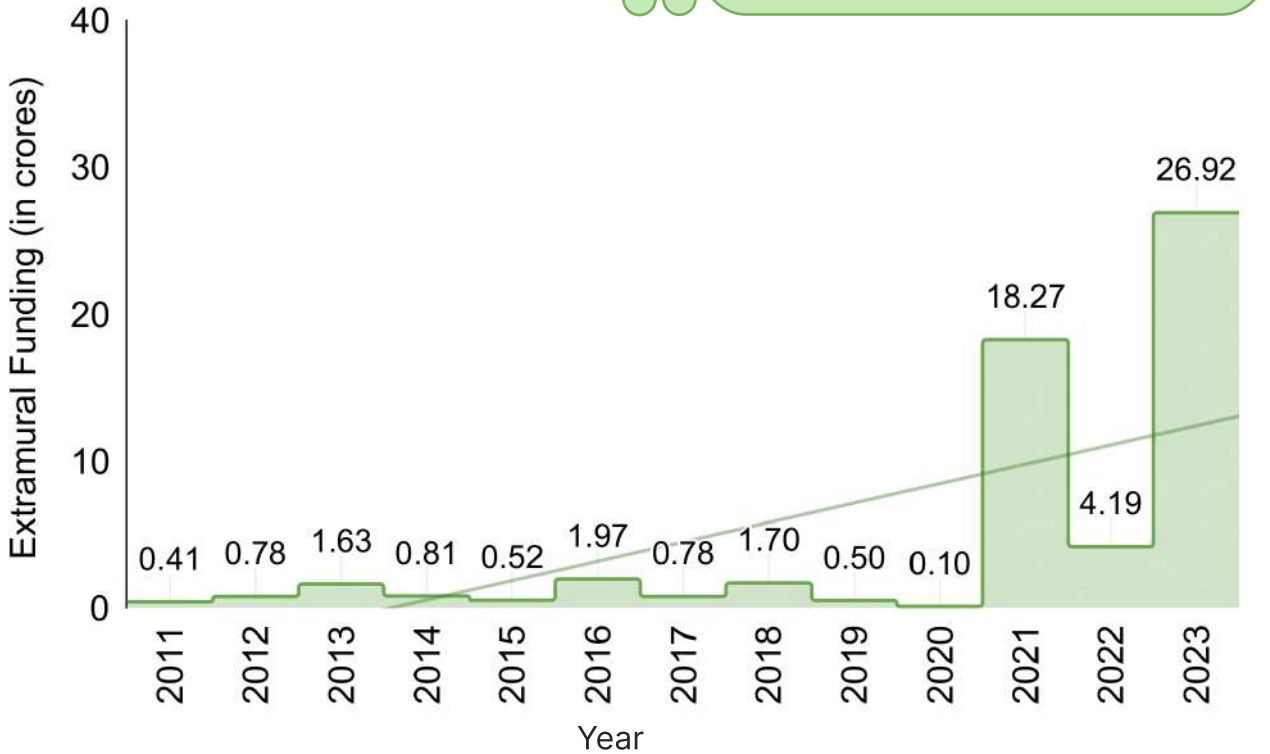


Research Publications and Funding

Publications



Sponsored Projects

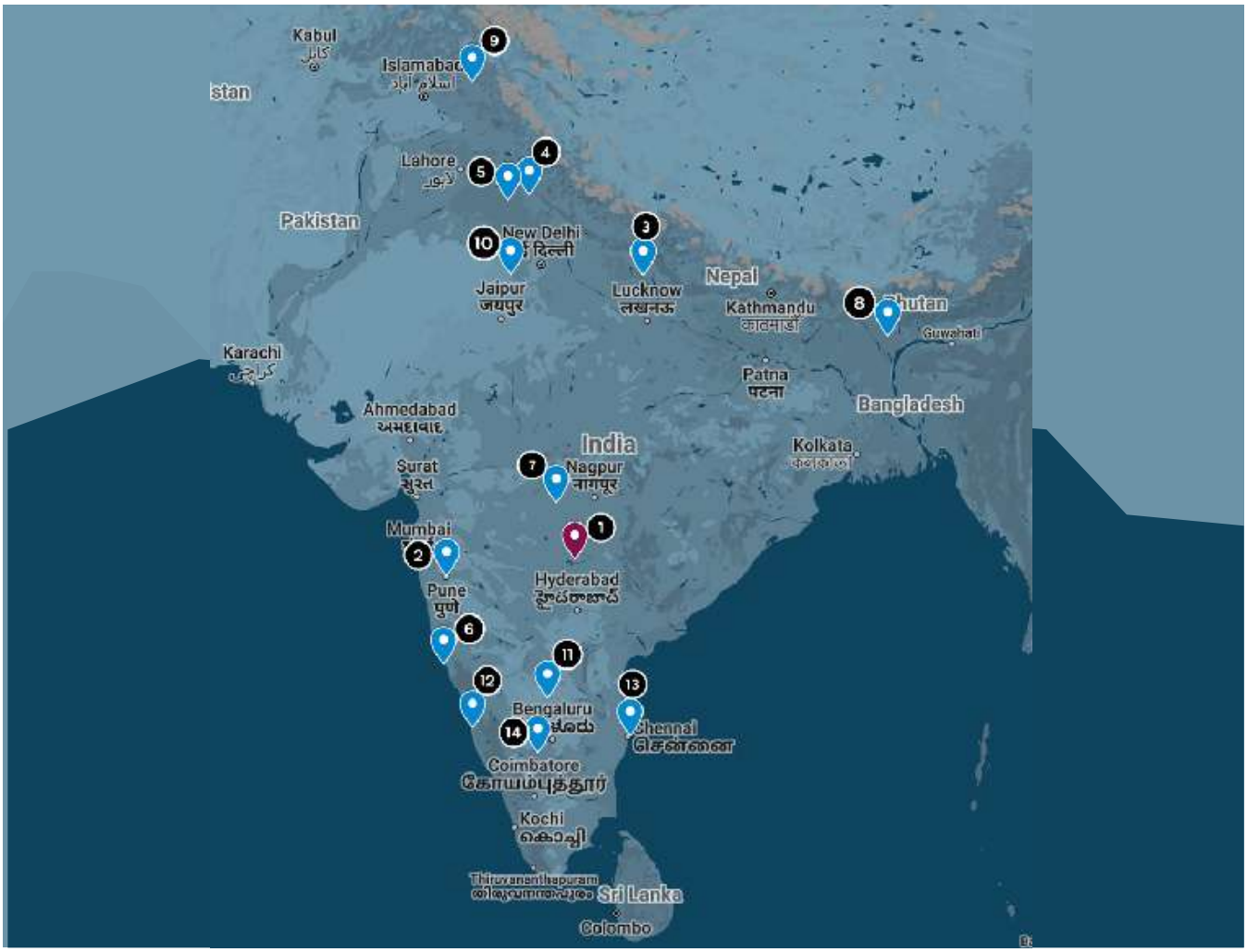



Building for
Department of Biotechnology and
Department of Biomedical Engineering

International Collaborations

Point	S.N.	Collaborator Name	Institute Name	Institute Country	Grant together	Publication together	Joint PhD together
1	1	Prof. Peter Carmeliet	VIB-KU Leuven Center for Cancer Biology	Leuven, Belgium		Yes	
2	2	Prof. Julia Gorelik	National Heart & Lung Institute, Imperial College	London, UK		Yes	
	3	Prof. Jann Scott	Newcastle University	UK	Yes		
3	4	Dr Andres Maturana	Nagoya University	Nagoya, Japan	Yes		
4	5	Dr. Salim Timo Islam	INRS-Institut Armand-Frappier Center	Quebec, Canada		Yes	Yes
5	6	Prof. Mitchell Singer	Dept. of Microbiology and Molecular Genetics, University of California	Davis, USA		Yes	
	7	Dr. Rebecca Parales		Davis, USA		Yes	
6	8	Prof. Emina A. Stojković	College of Arts and Sciences, Northeastern Illinois University	Chicago, Illinois, USA			
7	9	Dr. Pia H. Moisander	University of Massachusetts Dartmouth	Massachusetts, USA		Yes	
8	10	Prof. Akira Shinohara	Osaka University	Osaka, Japan	Yes		Yes
9	11	Prof. Dr. Ulrich Schwaneberg	RWTH Aachen University	Aachen, Germany		Yes	
10	12	Dr. Mehdi D. Davari	Leibniz Institute of Plant Biochemistry	Weinburg, Germany		Yes	
11	13	Prof. Simon Moulton	Swinburne University of Technology	Australia	Yes		
	14	Prof. Greg Murray		Australia	Yes		Yes
12	15	Prof. Richard Porter	University of Otago, Christchurch	New Zealand	Yes		

National Collaborations



Point	S.N.	Collaborator Name	Institute Name	Grant/s together	Publication/s together	Joint PhD together
1	1	Dr. Nagarajan Ganapathy	IIT Hyderabad			Yes
	2	Dr Shishir Kumar				Yes
	3	Dr. Rahul Kumar			Yes	
	4	Prof. T Shashidar				Yes
	5	Dr. Suhanya Duraiswamy		Yes		
	6	Dr. Satyavrata Samavedi				Yes
	7	Dr. Somnath Maji			Yes	
	8	Dr. Rajakumara Eerappa		Yes	Yes	Yes
	9	Dr. Aravind Kumar Rengan		Yes		Yes
	10	Dr. Krishna Guvvala		Yes		
	11	Prof. G. Satyanarayana		Yes	Yes	Yes
	12	Prof. Sumohana Channappayya				Yes
	13	Dr. Gunjan Mehta		Yes	Yes	Yes
	14	Dr. Jyotsnendu Giri		Yes	Yes	Yes
	15	Dr. Aravind Kumar Rengan,		Yes		
	16	Prof. Anindya Roy		Yes		
	17	Dr Swati Ghossh Acharyya	University of Hyderabad			Yes
	18	Dr. Vishal Rao	Indo-American Cancer Hospital, Hyderabad		Yes	
	19	Dr. Shweta Tyagi	CDFD, Hyderabad	Yes		
2	20	Dr. Ram Rup Sarkar	CSIR – NCL, Pune		Yes	
3	21	Prof. Nishant Verma	KGMU Lucknow	Yes		
4	22	Dr. Srikrishna Subramanian	CSIR-IMTECH, Chandigarh		Yes	
5	23	Dr. Rachna Chaba	IISER Mohali, Punjab			
6	24	Prof. Sanjeev C. Ghadi	Goa University, Goa			
7	25	Dr. Sutharsan Govindarajan	SRM University, Amarawati, AP			
8	26	Dr. Kapudeep Karmakar	UBKV, West Bengal		Yes	
9	27	Dr. Qazi Parvaiz Hassan	CSIR – IIIM, J&K			
10	28	Dr. Gunjan Goel	Central University of Haryana		Yes	
11	29	Dr. Kaustuv Sanyal	JNCASR, Bengaluru, KA		Yes	
12	30	Dr. Guruprasad Kalthur	Kasturba Medical College, Manipal, KA	Yes	Yes	
13	31	Dr. Athi N. Naganathan	IIT Madras, Chennai, TN	Yes		
14	32	Dr. P Ekambaram	Bharathiar University, Coimbatore, TN			

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Dr. Gaurav Sharma, BT-IITH

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