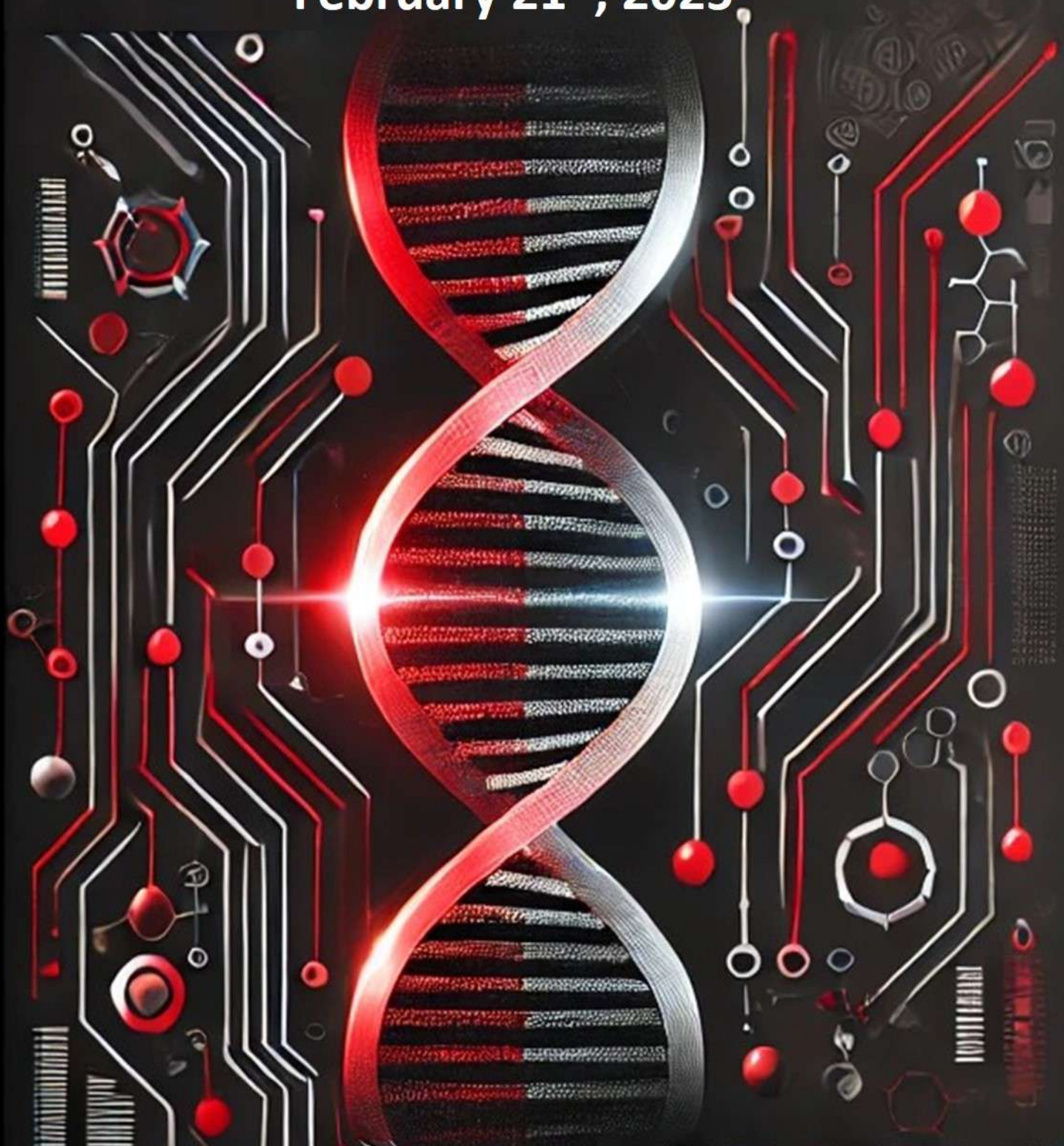
ONE-DAY SEMINAR ON SYNTHETIC BIOLOGY

February 21st, 2025



ABSTRACT BOOK

SVKM'S NMIMS Deemed to be UNIVERSITY

SUNANDAN DIVATIA SCHOOL OF SCIENCE

One Day Seminar on 'Synthetic Biology'

Organized by
Sunandan Divatia School of Science (SDSOS), SVKM's NMIMS (Deemed-to-be-University), Mumbai

In Collaboration with
Society of Biological Chemists India (SBCI), Mumbai Chapter

February 21st, 2025

ONE DAY SEMINAR ON 'SYNTHETIC BIOLOGY'

Organised by Sunandan Divatia School of Science,
SVKM's NMIMS (Deemed-to-be-University)
in collaboration with
Society Of Biological Chemists (India), Mumbai Chapter

21st February 2025 (Friday) | **8.30 a.m. to 5 p.m.**

Narsee Monjee Institute of Management Studies (NMIMS), established in 1981, is a premier academic institution of India. Conferred the status of a **"Deemed-to-be-University"** in 2003, NMIMS has grown into a multidisciplinary University with 17 constituent schools including **Sunandan Divatia School of Sciences (SDSOS)** along with Engineering and pharmacy schools and campuses across India. SDSOS started in 2007, offers academic and research programs focusing on **Biomedical Science, Chemistry and Physiotherapy**. The faculty at SDSOS comprises experts in various specialized fields such as Drug Discovery, Cancer biology, Nano-medicine, Cell and Molecular biology, Material Science, Energy etc.

PROSPECTIVE ATTENDEES

Students and faculties of NMIMS, University of Mumbai and affiliated Science colleges, HBSU, IITB, ACTREC, NIRRCH, BARC, TIFR, UDCT.

INVITED SPEAKERS

Dr. Smita Mahale
(Former Director, ICMR-NIRRCH Mumbai)

Dr. Debasis Das
(TIFR Mumbai)

Prof. Jacinta D'souza
(UM-DAE CEBS Mumbai)

Dr. Jomon Joseph
(NCCS Pune)

Dr. Prashant Phale
(IIT Bombay)

Prof. Birija S. Patro
(BARC Mumbai)

Dr. Jayeeta Giri
(DBT/Wellcome Trust Fellow ICMR-NIRRCH Mumbai)

Dr. Siddhesh Kamat
(IISER Pune)

Dr. Harinder Singh
(SDSOS NMIMS, Mumbai)

CONVENER (NMIMS)

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PROGRAMME SCHEDULE

'One Day Seminar on 'Synthetic Biology' organized by Sunandan Divatia School of Science, SVKM's NMIMS (Deemed-to-be) University, Mumbai in collaboration with Society for Biological Chemists (India), Mumbai Chapter	
Inauguration by Chief Guest (9.00 am to 9.30 am)	
Session 1	
Keynote Speaker **Prof. Smita Mahale**, Former Director, ICMR-NIRRCH, Mumbai **Title:** Structural and Functional Determinants of FSH Receptor: Implications in Female Reproduction	09.30 am to 10.15 am
Prof. Birija Sankar Patro, Head, Bio-organic Division, BARC Mumbai **Title:** CHK1-mediated regulation of TOP1 catalytic activity suppresses replication and transcription-associated genomic instability	10.15 am to 10.45 am
Prof. Debasis Das, TIFR, Mumbai **Title:** Defining a nascent protein conformation on the ribosome	10.45 am to 11.15 am
Tea break (11.15 am to 11.30 am)	
Session 2	
Prof. Jomon Joseph, Ph.D., NCCS, Pune **Title:** Understanding the Functions of an Underexplored Cell Organelle - Annulate Lamellae	11.30 am to 12.00 pm
Prof. Jacinta D'souza, CEBS, University of Mumbai **Title:** How Cells Move - Signalling Proteins to the Rescue!	12.00 am to 12.30 pm
Dr. Jayeeta Giri, NIRRCH, DBT/Wellcome-Trust fellow, NIRRCH, Mumbai **Title:** Adult stem cells in Female reproductive organ: Friend or Foe	12.30 pm to 01.00 pm
Doctoral Student Talk-1	1.00 pm to 1.10 pm
Poster Session and Lunch break (1.10 pm to 2.30 pm)	
Session 3	
Dr. Prashant Phale, Professor, Indian Institute of Technology Bombay **Title:** *Pseudomonas bharatica* CSV86^{T}: a promising host for metabolic engineering	2.30 pm to 3.00 pm
Prof. Siddhesh Kamat, Associate Professor, IISER Pune **Title:** An Integrated Metabolomics & Chemoproteomics Approach Towards Enzyme Function Annotation	3.00 pm to 3.30 pm
Dr. Harinder Singh, Assistant Professor, SDSOS, SVKM's NMIMS Deemed to-be University **Title:** Exploring the Role of Cold Shock Proteins in Bacterial Stress Tolerance	3.30 pm to 4.00 pm
Doctoral Student Talk-2	4.00 pm to 4.15 pm
Valedictory Function	4.15 pm to 5.00 pm
Tea and See Off	

Invited Speakers

S1 - Structural and Functional Determinants of FSH Receptor: Implications in Female Reproduction

Prof. Smita D. Mahale

Former Director,

ICMR-National Institute for Research in Reproductive and Child Health

Jehangir Merwanji Street, Parel, Mumbai 400012, India

Abstract:

Follicle stimulating hormone (FSH), a member of gonadotropin family is very crucial for mammalian reproduction. It is essential for ovarian folliculogenesis in females and spermatogenesis in males. It exerts its action by binding to specific receptor expressed on the plasma membrane of granulosa cells in the ovary and Sertoli-cells in the testis. Structural and molecular aspects of follicle stimulating hormone receptor (FSHR) with respect to ligand binding and signaling were investigated by employing various approaches like synthetic peptide, antipeptide antibodies, yeast two hybrid screens, site-directed mutagenesis etc. FSHR is a member of G-protein coupled receptor family and has an unusually large extracellular domain, which is believed to be involved in hormone recognition. Regions of FSHR involed in hormone binding, signal transduction have been delineated. Also the bionetralizing epitopes have been identified. This information will be useful in designing modulators of FSH which will have great application in developing targets of FSHR. We have also studied the interaction of FSH with its receptor in an in-vivo system, where the response of ovaries to FSH stimulation in women undergoing in-vitro fertilization (IVF) treatment is monitored. Some of the single nucleotide polymorphisms in the FSHR gene play an important role and association of two of them with altered ovarian response has been demonstrated. The polymorphism at 307 (Thr/Ala) is associated with hyper response and at -29 (T/A) is associated with hypo response. These findings indicate that the screening of FSHR genotype may be used to predict ovarian response in IVF clinics. Several novel/known mutations in FSHR gene have also been identified in infertile women and functional characterization of these mutants has been carried out using cell based assays. Methodology employed and results obtained will be discussed in detail.

S2 - CHK1-mediated regulation of TOP1 catalytic activity suppresses replication and transcription-associated genomic instability

Prof. Birija Sankar Patro

Head,

Bio-Organic Division
Dean (Acad) Life Sciences
Bhabha Atomic Research Centre (BARC),
Mumbai-400085, India

Abstract:

The Topoisomerase 1 (TOP1) catalytic cycle involves a TOP1-DNA-covalent-complex (TOP1cc), which, if stabilized, can induce rapid accumulation of potentially lethal DNA double strand breaks (DSBs). Although TOP1cc are critically associated with genome instability, it is not yet precisely known how cells regulate TOP1cc level, under unperturbed physiological-condition, to prevent its accumulation and lethal consequences. We discovered a key role of CHK1 in phosphorylating TOP1 at Serine-320 and stimulating TOP1-catalytic cycle to minimise genome wide accumulation of TOP1cc in cancers. Pharmacological or genetic ablation of CHK1-mediated TOP1- phosphorylation leads to stalled replication forks and generates copious amounts of replication/transcription-associated DSBs, R-loops and transcription-replication collisions, eventually leading to chromosomal instability. Further, TOP1ccs stabilized due to CHK1 inhibition are not efficiently targeted by cellular TOP1cc-removal machineries. Since multiple patient clinical trials are ongoing with TOP1- and CHK1- targeting drugs, current finding of CHK1-mediated regulation of TOP1cc may help in better understanding of the therapeutic outcomes

S3 - Defining a nascent protein conformation on the ribosome

Prof. Debasis Das
Reader, EMBO Global Investigator.
Department of Biological Sciences,
Tata Institute of Fundamental Research, Homi Bhabha Road,
Colaba, Mumbai 400 005, India

Abstract:

How does a newly synthesized protein start attaining its functionally active conformation, is unknown. That limits us to unravel molecular basis of nonfunctional protein production in cell, under pathological conditions. We are using a combination of biochemical, biophysical and cell biology approaches to explain protein folding mechanism of nascent sf-GFP (super folder GFP). Our results indicated that a population of full-length nascent sf-GFP yields functionally active structure while still attached to the last P-site tRNA at the PTC. The nascent protein sequence's regulated sequestration inside the peptide exit tunnel appeared crucial to form its functionally active conformation. The antibiotics known to affect translation elongation through their interaction with ribosomal RNA, reduced functional sf-GFP production, and the process is independent of peptidyl transferase action. The alteration of sf-GFPs redundant C-terminal amino acids significantly alters the puromycin labelled population of sf-GFP inside the living cell. An enhanced puromycin labelling showed a direct correlation with the significantly enhanced active sf-GFP population. The differential dwell time of individual nascent proteins on the ribosome presumably decides their functionally active population within the cell. Individual nascent proteins' characteristic dwell times on the ribosome allows them forming native intra-molecular contacts. A nascent protein can attain its native functional structure in its sequence dependent way, while still attached to the last P-site tRNA on the ribosome. The ribosome regulates this process independent of its peptidyl transferase activity.

S4 - Understanding the Functions of an Underexplored Cell Organelle - Annulate Lamellae

Prof. Jomon Joseph

Scientist G
National Centre for Cell Science
S.P. Pune University Campus
Pune – 411007, Maharashtra State, INDIA

Abstract:

Annulate Lamellae (AL) represent endoplasmic reticulum (ER) subdomains that harbour a subset of nucleoporins. Although this organelle was documented over 6-7 decades ago, its cellular functions have not been well understood. Research from our lab shows that AL could regulate the fate of cytoplasmic mRNAs and ER-mitochondrial functions.

S5 - How Cells Move - Signalling Proteins to the Rescue!

Prof. Jacinta S. D'Souza

UM-DAE Centre for Excellence in Basic Sciences,

School of Biological Sciences,

University of Mumbai, Kalina campus, Santacruz (E), Mumbai-400097

Abstract: Metazoans and several lower eukaryotic cells harbour one or more cilia and flagella, which are hair-like structures. These tubulin-based 9+2 architectures aid in motility and the perception of extracellular signals. My laboratory at CEBS has been using *Chlamydomonas reinhardtii*, an alga, and BCiNS cells (a human respiratory cell line) as model systems to study (1) the role of the central pair apparatus in the mechanism of motility, (2) the proteins involved in the formation of cilia, and (3) the involvement of human genes that cause primary ciliary dyskinesia, a disease resulting from dysfunctional cilia. Certain regulatory proteins and enzymes are destined for subcellular compartments to perform specific signalling roles in the form of signalosomes. A signalosome is a multiprotein complex that transmits signals between molecules within a cell. Each signalosome comprises unique combinations of components that are directed to specific locations in the cell. A-kinase anchoring proteins (AKAPs) act as scaffolds in a signalosome; these membrane-less subcellular assemblies are designed to sequester signalling proteins into subcellular compartments in microdomains. These modular structures are ubiquitous, vary in size, bind to the regulatory (RI or RII) and catalytic subunits of protein kinase A (PKA), and play crucial roles in cAMP-based signalling events.

In the quest to find the role of signalling proteins in cellular motility, our laboratory has identified four non-conventional AKAPs and two RII-like proteins in four different projections of the central pair apparatus of *Chlamydomonas* cilia. DPY-30 in C1a binds to PF16, and Myc-Binding Protein-1 orthologue (Flagellar Associated Protein 174, FAP174) in C2a, C1b, and C1d-e-f projections binds, respectively, to FAP65, CPC1, and FAP297. The non-conventional partners are currently being investigated for key features that will help understand the functioning of these signalosomes. The dimerisation and docking domain (aa 1-22) of FAP174 interacts with both the amphipathic helices of FAP65, an A-Kinase anchoring protein. The first 4 ASH domains of FAP65 interact with tubulin, a likely substrate for anchorage. FAP147, an orthologue of Myc-Binding Protein-Associated Protein (MycBP-AP), also binds to the C-terminus of FAP174. In addition, FAP147, although not a canonical protein kinase, exhibits PKA-like activity. Interestingly, FAP174 also binds to cAMP. This ternary complex from the C2a projection mimics the typical AKAP scaffolds spread across eukaryotic cells and facilitates cAMP-based signalling. In the C1b complex, FAP174 binds to another AKAP, CPC1 (central pair complex 1), with an adenylate kinase (ADK) domain. CPC1, in turn, binds to FAP42, yet another ADK, making this projection a probable hub of ATP homeostasis. FAP174 is also present in the C1d-e-f projection and is supported by the AKAP, FAP297. This complex is surrounded by Ca^{2+} and calmodulin-binding proteins, making this projection a Ca^{2+} signalling hub. PF16 in the C1a projection has been identified as an AKAP with DPY-30 as its RII-like partner. Taken together, the central pair apparatus likely uses cAMP-based signalling for mechano-transduction and maintaining the ATP pool.

S6 - Adult stem cells in Female reproductive organ: Friend or Foe

Dr. Jayeeta Giri

DBT Wellcome Trust Early Career Fellow,

ICMR-National Institute for Research in Reproductive and Child Health,

Indian Council of Medical Research (ICMR), Mumbai, India

Abstract:

The human uterine endometrium is an extremely dynamic tissue that suffers significant remodeling and regeneration on a fast and repeated basis, after parturition, menstruation, and injury. The capacity of the adult endometrium to undergo cyclic regeneration and differentiation/decidualization is essential for successful human reproduction. Impairment of the effective tissue regeneration process often leads to fibrosis. Endometrial stem cells (ESCs) are thought to play a major role in achieving this notable cellular turnover and tissue regeneration. Among ESCs, endometrial Mesenchymal Stem Cells are well characterized by their regenerative and immunomodulatory functionality. Nevertheless, only 1.25% of endometrial stromal cells exhibit clonogenicity, indicating a lower abundance of stem cells in the stroma. In my study, I hypothesized that the complex interplay between stem cells- derived secretomes, and immune cells, in the presence of reproductive hormones maintains tissue homeostasis during menstruation and embryo implantation. My study identified the fact that eMSCs-derived secretome has a significant impact on endometrial stroma remodeling during menstruation and embryo implantation

S7 - An Integrated Metabolomics & Chemoproteomics Approach Towards Enzyme Function Annotation

Dr. Siddhesh S. Kamat

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Indian Institute of Science Education and Research (IISER) Pune,
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Abstract:

Our research group is interested in studying the biological mechanisms of lipid signalling and metabolic pathways in the mammalian nervous and immune system. To achieve their goals, the group integrates aspects of chemical biology, biochemistry, molecular and cell biology, immunology, animal and/or cellular models, in conjunction with mass spectrometry (LC-MS) based metabolomics and proteomics techniques. The long-term goal is to identify and understand as-of-yet uncharacterized signalling and metabolic pathways *in vivo*, annotate enzymes and receptors that regulate their biology and provide new insights and therapeutic paradigms for various human diseases. In this talk, I will discuss our LC-MS based metabolomics and chemoproteomics approaches towards mapping functions to enzymes in a couple of physiological processes.

S8 - Exploring the Role of Cold Shock Proteins in Bacterial Stress Tolerance

Dr. Harinder Singh
Assistant Professor
Sunandan Divatia School of Science
SVKM's NMIMS (Deemed-to-be-University), Mumbai

Abstract:

Bacteria employ various mechanisms to withstand stress and adapt to changing environmental conditions. Cold shock proteins (CSPs) are a family of highly conserved proteins induced by low temperatures and other cellular stresses. They play crucial roles in maintaining cellular function under stress conditions by binding to single-stranded RNA and DNA, influencing mRNA translation, and regulating gene expression. Beyond cold shock, CSPs contribute to tolerance of osmotic, oxidative, starvation, pH, and ethanol stress. They achieve this through chaperone and regulatory functions that maintain cell membrane fluidity, enzyme activity, and gene expression. Some CSPs are non-cold inducible, suggesting their involvement in normal growth, metabolism, virulence, and adaptation to various stress conditions. Furthermore, the overexpression of CSPs has demonstrated improved stress tolerance in bacteria. This exploration of CSPs highlights their importance in bacterial stress tolerance and adaptation, providing insights into their structure, function, and regulatory mechanisms, and inspiring future research into their potential biotechnological and biomedical applications.

S9-Molecular mechanisms underlying the nucleoid organization in *Deinococcus radiodurans*

Shruti Mishra[1,2]

[1] *Molecular Biology Division, Bhabha Atomic Research Centre, Mumbai-400085.*
[2] *Life Sciences, Homi Bhabha National Institute, Mumbai- 400094.*
Scientific Officer-D, *email-mshruti@barc.gov.in*

Abstract:

Deinococcus radiodurans, an extremely radioresistant coccus bacterium, withstand around 15 kGy dose of radiation, i.e. about 3000 times the radiation tolerance of humans. Its highly efficient DNA damage repair mechanism and unique genome arrangement are some of the factors responsible for this extraordinary radioresistant phenotype. This bacterium contains a polyploid multipartite genome, which is tightly packaged in the form of a doughnut-shaped toroidal structure. How this unique genome organization is maintained is still unknown. In other bacterial systems, chromosome dimers are formed after replication due to homologous recombination between the sister chromosomes. In *D. radiodurans*, polyploidy increases the chances of the formation of chromosome dimers. So, how these dimers are resolved and whether that has any significance to radiation resistance in this bacterium are the most intriguing questions. The chromosome dimer resolution system involves the function of site-specific tyrosine recombinases (Xer) that could function independently or by the activation from the FtsK protein.

Bioinformatics analysis has revealed that *D. radiodurans* encodes FtsK and six putative tyrosine recombinases, indicating the existence of a functional site-specific recombination (SSR) system. We have earlier demonstrated the functional activity of DrFtsK *in vitro.* We created different domain disruption mutants of *ftsK* and one of the putative tyrosine recombinase (*dr0513*), and these mutants showed many abnormalities at the nucleoid levels. Mutants also exhibited increased generation time than the wild type in normal conditions and post-gamma irradiation. Our findings highlight the role of SSR in maintaining the unique nucleoid architecture of *D. radiodurans.*

S10-Chrysin Ameliorates Adverse Effects of Therapy-Induced Senescence in Breast Cancer by Attenuating cGAS-STING pathway

Rezina Billimoria and Purvi Bhatt*

Department of Biological Sciences, Sunandan Divatia School of Science,

SVKM's NMIMS (Deemed-to-be University), Vile Parle (West), Mumbai, India.

Abstract:

Breast cancer is the most prevalent cancer among women globally, with recurrence posing a significant challenge despite various treatment options. One major contributor to cancer recurrence is therapy-induced senescence (TIS), where prolonged exposure to chemotherapy forces cancer cells into a senescent state. Senescent cells enter permanent growth arrest but secrete pro-inflammatory cytokines and chemokines, collectively known as the senescence-associated secretory phenotype (SASP), which promotes tumour progression by altering the surrounding tissue environment and fostering angiogenesis. The rejuvenation of senescent cells from this state can lead to more aggressive and malignant tumour behaviour. Targeting SASP may, therefore, be a crucial therapeutic strategy to reduce cancer recurrence. The SASP is largely driven by the activation of the cGAS-STING pathway, triggered by cytoplasmic chromatin fragments (CCFs) within senescent cells, which release inflammatory cytokines such as IL-6 and IL-8. Chrysin, a natural flavonoid predominantly found in propolis and honey, has shown strong antioxidant and anti-inflammatory effects. In this study, we investigate chrysin's ability to modulate the SASP in senescent breast cancer cells, particularly focusing on its impact on CCF markers H3K9me3 and H3K27me3. Senescent breast cancer cells were analysed for the expression levels of inflammatory cytokines IL-6 and IL-8 following treatment with varying concentrations of Chrysin through qRT-PCR. A significant reduction in CCF markers H3K9me3 and H3K27me3, alongside decreased STING phosphorylation, was observed after chrysin treatment. Notably, Chrysin did not alter senescence markers such as p16, p21, or BCL-2, indicating it does not trigger apoptosis. Additionally, Chrysin effectively inhibited SASP-driven breast cancer cell invasion and colony formation, underscoring its potential as both an anti-inflammatory agent and a senomorphic drug. Chrysin acts as a senomorphic drug by attenuating the cGAS-STING pathway, thereby reducing SASP-mediated inflammation in breast cancer cells. This suggests Chrysin's therapeutic potential in mitigating the pro-tumorigenic effects of cellular senescence, offering a novel approach to treating breast cancer.

Keywords: Senescence, Senomorphic Drug, SASP, chrysin, CCF

S11- Modeling signal flow variability for ensemble-level regulation of cancer cells

Shubhank Sherekar, Chaitra S Todankar, Ganesh A. Viswanathan*

Department of Chemical Engineering

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Abstract: Cells respond heterogeneously to external environment. Cell-to-cell variability during TNFα stimulated TNFR1 signaling system can lead to single-cell level pro-survival and cell-death responses. This variability stems from the heterogeneity in signal flow through intracellular signaling entities within and across cells that regulate the balance between these two phenotypes. However, cancer cells shift the signal flow towards survival during TNFα stimulation. Modulating the variable signal flow to enable cells favor apoptosis, an important paradigm considered in cancer therapies, is still under investigation. Using systematic Boolean dynamic modeling of TNFR1 signaling network accounting forsignal flow path variability, we revealed crucial dynamic cross-talk regulation between pathways that may be regulating these two phenotypic responses at single-cell level. We developed a computationally efficient approach "Boolean Modeling based Prediction of Steady-state probability of Phenotype Reachability (BM-ProSPR)" to accurately predict the network's ability to settle into different phenotypes. Model predicted the experimentally observed long term response of multiple cell lines. We further showed that arresting TAK1 activity can re-wire the signal flow paths towards apoptotic response without severely hampering the essential actions of a cell. Strikingly a ~31% increase in apoptotic response matched well those observed in U937 cells exposed to TAK1 inhibitor which mediates the complex between Comp1 and IKK∗ . Modulating the casual mechanisms in cancer cells by rewiring signal flow via upstream nodes/interactions could be a potential therapeutic strategy.

Poster Abstracts

P1 - Title: Kinase associated Serine/Threonine-Specific Phosphatase implications in radiation and oxidative stress resistance of *Deinococcus radiodurans.*

Ishu Soni*, and Yogendra Singh Rajpurohit

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Abstract:

Deinococcus radiodurans is renowned for its extreme tolerance to radiation and oxidative stress, a trait attributed to a suite of protective mechanisms. These include exceptionally effective DNA double-strand break (DSB) repair, protection of DNA and proteins against oxidation, and strong antioxidant defenses. Different from many bacteria, like the widely studied *E. coli*, *D. radiodurans* lacks the typical SOS repair pathway, as it does not possess LexA-mediated transcriptional activation of SOS regulon genes. Instead, it utilizes Serine/Threonine (S/T) phosphorylation to regulate cell division and DNA repair, primarily through a radiation-sensitive S/T protein kinase (STPK) called RqkA. This research biochemically characterized DR_A0334, a kinase-associated S/T-specific protein phosphatase (STPP) from *D. radiodurans*, by creating active site mutants and examining their biochemical properties. We further show that DR_A0334 can dephosphorylate RqkA and other identified phosphoproteins. Moreover, overexpressing this phosphatase constitutively improves survival under stress from DNA-damaging agents. Comprehensive data and findings will be shared.

Keywords: RqkA, STPP, STPK oxidative stress

P2 – Title: Revolutionizing Drug Discovery with Quantum Computing: Techniques, Challenges, and Emerging Potential

Virendra S. Gomase*[1,2], Rupali Sharma[2] and Suchita P. Dhamane[3]

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[2]Department of Pharmaceutics, Jayawantrao Sawant College of Pharmacy and Research, Savitribai Phule Pune University, Pune, 411028, India

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Abstract:

The use of quantum computing to develop drugs is revolutionizing the industry by providing previously unimaginable potential for improving drug design and modeling intricate chemical interactions. It is possible to save time and expense using the conventional approach significantly, and researchers can identify drug candidates much quicker, with quantum algorithms like Grover's algorithm and the Variational Quantum Eigensolver. However, various technology hurdles against implementing quantum computing into pharmaceuticals include error limits on rates and coherence of qubits, difficulties with data and compliance with the regulatory framework. The pharmaceutical sector is presented with enormous opportunities due to the ability of quantum computing to enhance drug design, facilitate personalized therapy, and foster interdisciplinarity, in spite of these challenges. The utility of quantum technologies is illustrated using case studies, for instance, IBM's application of the Variational Quantum Eigensolver (VQE) for molecular simulations that highlight successful applications demonstrating how effective they are in addressing real drug development challenges. Quantum algorithms and technology paving the way for widespread pharmaceutical application. Quantum computing is likely to make a big difference in drug development in the future, leading to quicker, more effective treatments and a shift in paradigm in the design and delivery of new therapeutics. Quantum computing has promise in drug development and discovery, particularly in multifaceted fields such as protein folding, prediction, and personalized medicine. Aside from examining the challenges faced, this essay points to new opportunities that can potentially revolutionize the pharmaceutical sector.

Keywords- Quantum Computing, Drug Discovery, Quantum Algorithms, Molecular Simulation, Challenges, Emerging Opportunities, Personalized Medicine, Pharmacogenomics

P3 – Title: Understanding the Differential Binding Affinity of Katanin Hexamer with different β-tubulin Isotypes using molecular modeling approach

Vibhuti Saxena, Pruthanka Patil and *Bajarang Vasant Kumbhar**

Department of Biological Sciences, Sunandan Divatia School of Science, SVKM's NMIMS (Deemed-to-be University), Mumbai.

Email: Bajarang.Kumbhar@nmims.edu

Abstract:

Katanin, a microtubule-severing ATPase, plays a crucial role in cytoskeletal dynamics by regulating microtubule disassembly. It exists as a monomer but functions in a hexameric state. Microtubules are composed of αβ-tubulin heterodimers, with nine α-tubulin and ten β-tubulin isotypes exhibiting tissue-specific expression. The activity of katanin is modulated by its differential binding affinities to the C-terminal tails of several β-tubulin isoforms, including βI, βIIa, βIIb, βIII, βIVa, and βIVb. Notably, these isotypes are highly expressed in cancerous cells and are involved in key cellular processes such as cell division, intracellular transport, and chemoresistance. However, the precise binding mode and affinity of hexameric katanin for the β-tubulin C-terminal tail remain unclear at the atomic level.

In this study, we employed protein modeling, hexamer assembly, and molecular docking simulations to investigate the selective binding affinity of human katanin hexamer with various β-tubulin isotypes. Our findings reveal that katanin exhibits differential binding affinities, with the highest affinity observed for βII- and βIII-tubulin, followed by βIVa, βIVb, and βI. This suggests a potential role of katanin in enhancing microtubule severing in cancer cells, where these isotypes are predominantly expressed. Moreover, the negatively charged C-terminal tail of β-tubulin was found to be a critical determinant of katanin's severing efficiency by facilitating electrostatic interactions and protein accessibility. These insights provide a comprehensive understanding of the molecular determinants governing katanin-tubulin specificity and offer potential avenues for targeting microtubule dynamics in cancer therapy.

Keywords: Cancer, Katanin, Microtubule, molecular docking, binding affinity

P4 – Title: Computational Development of a Phytochemical Repository For Potential Anti-Arthritic Drug Candidates

Namrata Britto[1], Rajasekhar Reddy Alavala[2], *Brijesh S.[1]*

[1]Sunandan Divatia School of Science, NMIMS, Mumbai

[2]Shobhaben Pratapbhai Patel School of Pharmacy & Technology Management, NMIMS, Mumbai

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Abstract:

Arthritis is a progressive and debilitating condition affecting millions worldwide with limited treatment options that often pose adverse effects. Phytochemicals derived from medicinal plants offer a promising avenue for drug discovery due to their diverse bioactive properties. This study focuses on the development of a phytochemical database to identify potential drug candidates for various types of arthritis through a systematic computational approach. A curated library of phytochemicals was compiled from various sources and analyzed for drug-likeness and ADMET properties using SwissADME and Protox 3.0 respectively. The results provide a comprehensive database of phytochemicals with favorable pharmacokinetic profiles and potential therapeutic activity against arthritis. The source serves as a foundation for further experimental validation and optimization of phytochemical-based therapeutics. Future studies will focus on confirming the bioactivity of lead compounds through in vitro and in vivo models along with formulation strategies to enhance their efficacy.

P5 – Title: Cas11 augments Cascade functions in type I-E CRISPR system but is redundant for gene silencing and plasmid interference

Neha Pandey[1,2], *Chitra S Misra*[1], and *Devashish Rath*[1,2]

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[2]Life Sciences, University of Mumbai, Mumbai- 400001

Department of Science and technology India

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Abstract:

The structural and mechanistic complexity of *Escherichia coli*'s type I CRISPR-Cas system compared to the multidomain, single effector protein-based type II systems, limits its application in genome editing and silencing. Despite higher prevalence of the type I endogenous systems in bacteria, significant research has focused on improving the type II systems. While the type-I CRISPR system possesses several advantages over others, it may benefit from further studies to simplify the system for ease of use. To enable this, the dispensability of the type-I Cascade components (Cas8, Cas11, Cas7, Cas5, Cas6) for genome editing and silencing applications was evaluated in vivo. We created deletion variants of each of the Cascade components and investigated their effects on gene silencing and plasmid interference in two *Escherichia coli* lineages, BW25113, a K-12 strain that bears an endogenous, albeit repressed type I-E CRISPR system and BL21, a natural mutant lacking the type I-E CRISPR-Cascade system. Cas8, Cas7 and Cas5 were found to be indispensable for gene silencing and plasmid interference. Dispensability of Cas6, which is involved in crRNA maturation, was strain-dependent. Notably, Cas11 which has no definitive function assigned to it, was found to be dispensable for gene silencing and plasmid interference.

Keywords: Cas11, Gene silencing, Plasmid interference, Minimal cascade.

P6 – Title: Decoding Telomeres in Age Related Diseases

Meghna Jain, *Ekta Khattar**

Sunandan Divatia School of Science, SVKM's NMIMS (Deemed to be) University, Mumbai, India.

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Abstract:

Telomeres are repetitive DNA sequences play a crucial role in maintaining genomic stability and are located at the ends of chromosomes. As we age, telomeres gradually shorten due to the limited activity of the enzyme telomerase. This shortening has been associated with an increased risk of various diseases. In our study, we investigated telomere length in blood samples collected from individuals across different age groups. Our findings consistently revealed a decline in telomere length with advancing age. Notably, we observed gender specific differences, with females exhibiting longer telomeres than males as they grew older. Of particular interest is the link between age-related diseases and telomere length. Diabetes, a prevalent condition affecting millions worldwide, has been associated with shorter telomeres. Oxidative stress, a hallmark of diabetes, accelerates telomere attrition. Additionally, chronic inflammation, common in diabetes, further contributes to telomere shortening. Diabetes, a prevalent condition affecting millions worldwide, has been associated with shorter telomeres. Oxidative stress, a hallmark of diabetes, accelerates telomere attrition. Additionally, chronic inflammation, common in diabetes, further contributes to telomere shortening. In summary, understanding the intricate relationship between telomeres, diabetes, and age-related diseases is essential. Further research exploring novel therapeutic targets may pave the way for interventions that promote healthy aging and prevent disease progression.

P7 – Title: First-in-class clinical candidate ONC201 inhibits proliferation of cervical cancer cells by triggering integrated stress response

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Abstract: Cervical cancer is second most commonly occurring cancer in women in India and is third leading cause of deaths in women globally. Prophylactic treatment is effective only if administered before the first exposure to Human Papillomavirus (HPV) infection. Systemic chemotherapy is a standard treatment for advanced stage disease with poor prognosis but provides only limited therapeutic benefit due to toxicity and drug resistance.

ONC201 (also known as TIC10), is a TRAIL (TNF-Related Apoptosis Inducing Ligand) and cIpP (caseinolytic protease) agonist with proven efficacy in various preclinical models and is currently in Phase II clinical trials for different types of cancer. In the present study, we investigated the anticancer potential of ONC201 in HPV-positive cervical cancer cell lines - HeLa and SiHa. ONC201 exerted significant cytotoxicity and inhibited clonogenic potential of these cells. It induced integrated stress response followed by S/G2-M arrest and apoptosis in both cell lines. Yet, surprisingly, well-known targets of ONC201 viz. TRAIL, DR5 (death receptor 5) and cIpP were found to be upregulated in HeLa but not in SiHa cells. In addition, expression levels of BNIP3 and Beclin-1 (involved in regulation of autophagy) increased in response to certain doses of ONC201. ONC201-induced cell cycle arrest and apoptosis were independent of p53. Furthermore, ONC201 exhibited synergism in combination with standard drugs against cervical cancer cells. This study provides proof-of-concept for anticancer activity of versatile drug ONC201 and also delineates its mechanism of action.

Keywords: ONC201, cervical cancer, dordaviprone, apoptosis, integrated stress response

P8 – Title: Glycoxidation-Driven Oxidative Stress and cAMP Dysregulation in Diabetes: A Case Study

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Abstract:

Diabetes mellitus is defined by persistent hyperglycemia that causes oxidative stress and stimulates advanced oxidation protein product (AOPP) and fluorescent advanced glycation end-product (fAGE) generation through glycoxidation. Such oxidative markers contribute to vascular and metabolic complications, emphasizing the role of oxidative stress in diabetes pathogenesis. Cyclic adenosine monophosphate (cAMP), located within cells, is important for modulating oxidative stress and inflammation, possibly playing a role as a diabetes-associated metabolic function modulator. The aim of this study, on 30 individuals (11 women, 19 men), was to determine biochemical parameters, including HbA1c, lipid levels, AOPPs, fAGEs, and cAMP, using fluorescence tests and immunoenzymatic test. Patients had greater levels of fAGE levels (34.7 ± 1.2) compared to diabetes of ≤5 years' or 5- to 10-year durations (19.7 ± 1.2 or 24.7 ± 1.5, $p < 0.05$), indicating that disease duration is greater among individuals with greater levels of disease severity. HbA1c had a good relationship with cAMP ($r = 0.859$, $p = 0.0002$), whereas there were good relationships of fAGEs with markers of oxidative stress, N-formylkynurenine ($r = 0.9233$), and dityrosine ($r = 0.9508$). Regression modeling demonstrated that 73.8% of variance of cAMP is explained by HbA1c levels ($R^2 = 0.7379$). The findings of this study reflect on how complex is the relationship of glycoxidation products to cAMP signaling, pointing to possible avenues of therapy targeting diabetes through pathways of oxidation.

Keywords: Glycoxidation, Oxidative stress, Advanced glycation end-products (AGEs), Cyclic adenosine monophosphate (cAMP), Diabetes mellitus

P9 – Title: Generation and characterization of CRISPR-cas9-mediated Flag POT1 gene knock-in

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Abstract:

POT1 (Protection of Telomeres 1) is the only single-stranded telomere-binding protein in the Shelterin complex. Together with TPP1, POT1 plays a crucial role in regulating telomere length and protecting telomeres from DNA damage repair proteins. The activation of DNA damage repair proteins at telomeres can be detrimental to cells, so their activity must be suppressed. This suppression is achieved through a group of proteins known as the Shelterin complex. POT1 interacts with other Shelterin proteins via its association with TPP1. These Shelterin proteins function together to protect and maintain the telomeres. Telomeres shorten due to the end replication problem, but this issue is addressed in germ cells and cancer cells by the enzyme telomerase. Research has shown that POT1 inhibits telomerase binding to telomeres. Additionally, POT1 recruits the CST-STN complex for 5' resection. Loss-of-function mutations in the POT1 gene lead to telomere elongation, resulting in the accumulation of telomere dysfunction-induced foci (TIFs). In our study, we generated an endogenous Flag-tag knock-in of the POT1 gene using CRISPR-Cas9, without disrupting its functional characteristics related to telomere and TPP1 binding. During our screening, we identified two additional clones that also contained the Flag sequence and protein, but exhibited an increase in telomere length. Furthermore, we analyzed the proteome of the Flag-tagged POT1 in the chromatin fraction of clone. Our screening and characterization of this clone provide a comprehensive understanding of the molecular and functional characteristics of POT1.

Keywords: CRISPR, Telomeres; POT1; genome instability; cancer; DNA Damage

P10 – Title: Metabolic engineering of *Pseudomonas bharatica* CSV86 for the production of bioplastic (poly-3-hydroxybutyrate)

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Abstract:

The use of plastic is ever-increasing with the rise in human population. Despite several advantages, plastic takes hundreds of years to degrade. Additionally, plastic monomers and plasticizers used in plastic manufacturing are known to cause cytotoxicity, mutagenicity and endocrine disruption. Therefore, it is crucial to address the harm caused by plastics and find a sustainable alternative. Bioplastics, particularly poly-3-hydroxybutyrate (PHB), offer a solution with properties similar to conventional plastics and are biodegradable. However, high production costs hinder its commercialization. To address this challenge, we can engineer an organism which utilizes pollutants as carbon source and convert them into bioplastic. *Pseudomonas bharatica* CSV86^T, a robust bacterial strain that preferentially degrades aromatic compounds over simple carbon sources like glucose, can be employed for bioremediation. CSV86 degrades wide range of aromatic compounds and funnel them into central carbon intermediates mainly, acetyl-CoA. Acetyl-CoA is a direct precursor for PHB synthesis. In this study, we engineered *P. bharatica* CSV86^T for the production of poly-3-hydroxybutyrate (PHB) by cloning genes for PHB synthesis. The PHB biosynthesis genes were cloned from *Cupriavidus necator* H16 and expressed under the p*trc* and a host-specific promoter, p*nah*, in the pSEVA vector. These vectors were electroporated into CSV86, and the transformants were assessed for their ability to produce PHB using naphthalene (aromatic pollutant) as a substrate. The PHB production was assessed by the Nile red plate assay, and it was found that heterologous expression of *pha*CAB gene cluster rendered strain CSV86^T capable of producing PHB using naphthalene as sole carbon source.

Keywords: Metabolic engineering, Aromatic degradation, Bioremediation, Poly-3-hydroxybutyrate.

P11 – Title: Plant growth promoting and biocontrol attributes of aromatic degrading *Pseudomonas* and *Acinetobacter*

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Abstract:

Aromatic compounds are extensively used in agricultural products like insecticides herbicides, fungicides, mulching films *etc.* These compounds are mutagenic, endocrine disrupting, carcinogenic and are known to have non-target toxicity leading to compromised soil health and crop production. In this study, five soil bacteria *viz. Pseudomonas bharatica* CSV86^T, *Pseudomonas* sp. C5pp, *Pseudomonas* sp. PP4, *Pseudomonas* sp. PPD and *Acinetobacter* sp. ISP4 that efficiently degrades various aromatic compounds like naphthalene, Carbaryl, phthalate isomers, *etc*. were found to be effective plant growth promoters. These strains possess ability to solubilize inorganic minerals (P & K) and to produce IAA, ammonia and siderophores. Seed priming of wheat, mung bean and fenugreek with individual strains or their consortium resulted in significant increase in seedling shoot length (15-37%), root length (65-150%) and biomass (30-40%). Moreover, the antifungal activity against phytopathogenic fungi *Magnaporthe oryzae* and *Aspergillus* spp. revealed their biocontrol potential. The biofilm formation ability as consortium, fusaric acid resistance (1-1.2 mg. mL^{-1}) and salinity tolerance (5-7.5%) indicates their niche colonisation potential at site. Presence of aromatic compounds in soil (spiked with 250 or 1000 ppm each of naphthalene, Carbaryl, terephthalate and isophthalate) lead to phytotoxicity including inhibition of seed germination (32-67%) and seedling growth (34-65%) of mung bean. Seed priming with consortium released (up to 25-100%) toxicity of aromatics to mung bean seedlings. The four aromatics degrading bacteria exhibits plant growth promoting as well as biocontrol activity and has potential to be used as a tri-purpose consortium as bioremediators-biofertilizer-biocontrol agent for sustainable environmental clean-up and crop production.

Keywords: Aromatic degradation, Plant-growth-promotion, Consortium, Bioremediation, Biocontrol.

P12 – Title: Boosting fatty acid production using heterogenous regulator for diverse applications

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Abstract:

Since 1900s, fatty acid (FA) production has drawn immense industrial attention due to its diverse application. These acids are harvested from various oleaginous sources like plants, algal and fungal species. However, researchers are in search of alternatives to these sources due to their inherent shortcomings. Also, the various stresses generated due to/during FA production adds on the burden limiting its own potential to overproduce FA. In this study, a *Deinoccocal* response regulator DR1558 was cloned in an *E. coli* mutant strain (Δ*fadD*), *E. coli* Δ*fadD*-1558 rendering multi-stress tolerance. The final Δ*fadD*-1558 strain not only produced 1.75 times higher FA titers (85mg/L FA) than the control strain but also restored the growth rate as compared to the other strains.

P13 – Title: Computational Analysis of Calcium Dysregulation in Neurodegenerative Diseases

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Abstract:

Calcium plays an important role in presynaptic and postsynaptic transmission of neuronal signalling. Calcium homeostasis is significant in synaptic plasticity and neuronal protection. Overload of the calcium inside the mitochondria leads to cell death observed in neurodegenerative disorders like Alzhiemer, Parkinsons and Huntington. Calcium dysregulation leads to an imbalance in reactive oxygen species (ROS), thereby affecting mitochondrial membrane potential. This effect is further observed in dysregulation of PINK1 (in Parkinsons), PSEN (in Alzheimer's) and mHTT (in Huntington) dysfunction. Dysregulation of these proteins directly influences mitochondrial calcium uptake. Computational tools can be used to evaluate these damages.

The analysis of transcriptomics data from NCBI- GEO will reveal differentially expressed genes (DEGs) linked to calcium homeostasis. Mechanisms of disease neurodegeneration can be attained by mapping these genes to neurodegenerative signaling networks using KEGG pathway enrichment. STRING and Cytoscape will be used to make a protein- protein interaction (PPI) network in order to find important relations between the proteins. These computational tools will help us to comprehend Ca2+ effect on multiple neurodegenerative pathways across these three diseases. Finding new remedial targets and corrective measures to restore calcium homeostasis and decelerate the course of neurodegeneration may be made easier with the computational tools followed by experimental datasets.

P14 – Title: Discovery of natural compound inhibitor against drug-resistant human αβIII Tubulin Isotype Using Virtual Screening, Machine Learning, and Molecular Dynamics Simulations.

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Abstract:

Microtubules (MTs) play a crucial role in mitosis and are composed of α-/β-tubulin heterodimeric subunits. In eukaryotes, eight α-tubulin and ten β-tubulin isotypes have been identified, each displaying tissue-specific expression patterns. Among them, the βIII-tubulin isotype is significantly overexpressed in various cancers and is closely associated with resistance to anticancer agents, making it an attractive target for cancer therapies. This study employed a comprehensive pipeline integrating structure-based drug design, machine learning, ADME-T and PASS property evaluations, molecular docking, and molecular dynamics simulations to identify potential natural compounds targeting the 'Taxol site' of the αβIII-tubulin isotype. Screening 89,399 compounds from the ZINC natural compound database yielded 1,000 initial hits based on binding energy. Refinement using machine learning classifiers narrowed these to 20 active compounds, of which four - ZINC08952577, ZINC08952607, ZINC12889138, and ZINC03847075 exhibited exceptional ADME-T properties and notable anti-tubulin activity. Molecular docking revealed significant binding affinities of these compounds to the 'Taxol site' of αβIII-tubulin isotype. Molecular dynamics simulations, assessed through RMSD, RMSF, Rg, and SASA analyses, demonstrated that these compounds notably impacted the structural stability of the αβIII-tubulin heterodimer comparing to the apo form of αβIII-tubulin isotype. Binding energy calculations confirmed that ZINC08952577 exhibited the highest binding affinity, while ZINC03847075 showed comparatively lower affinity. In conclusion, this study successfully identified natural compounds with potential anticancer activity against the human αβIII-tubulin isotype. These findings provide a strong foundation for developing innovative therapeutic strategies targeting carcinomas characterized by βIII-tubulin overexpression.

Keywords: β_{III}-tubulin, anti-cancer, Virtual screening, Machine learning, MD Simulation

P15 – Title: Network Pharmacological Analysis of secondary metabolites from *Mammea suriga* (Buch.-Ham. ex Roxb.) Kosterm. targeting Eczema

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Abstract:

This project aims to identify and characterize bioactive compounds from *Mammea suriga* (Buch.-Ham. ex Roxb.) Kosterm. (a coastal tree native to south India) with potential therapeutic activity against Eczema. Using bioinformatics tools, phytochemicals identified from the stem of Mammea were investigated for their structure and effect in disease pathways. Network pharmacology encompasses the study of the effect of a compound on the entire network, rather than the traditional one drug-one target approach of drug discovery. The bioactive compounds were analysed with Gene Ontology and KEGG pathway enrichment. The compounds will subsequently be embedded into a protein-protein interaction (PPI) network to elucidate their molecular targets and mechanisms of action. The PPI network, constructed using publicly available interactome data, will integrate compound-gene product interactions to identify key regulatory nodes affected by the compounds. Network pharmacology analyses will be employed to predict pathways modulated by the compounds, identify synergistic effects, and evaluate their therapeutic potential. This systems-level approach will provide insights into the molecular basis of eczema and aid in the rational design of new drug therapy strategies.

Keywords: Network pharmacology, Mammea, protein-protein interaction (PPI), Eczema

P16 – Title: Design of Fully Human CAR-scFv Against Membrane Bound CD20 for B Cell Malignancies Using Molecular Modeling Approach

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Abstract:

CAR-T cell therapy involves genetically modifying T cells with synthetic receptors to target and eliminate cancer cells. Yet challenges with respect to the use of chimeric monoclonal antibodies (mAbs) for scFv derivation remain, which can cause damage to the CAR-T cells themselves. To address it, human mAbs act as a promising alternative. Currently, FDA approved CARs are available for CD19 & BCMA antigens. Despite CD20's overexpression on malignant B-cells, CAR therapies targeting it remain under development. Being a membrane proximal antigen with short epitope regions, it becomes challenging for CAR to bind with CD20, resulting in shorter residence time, leading to treatment failure. Hence for overcoming this, we have used computational approach to design CAR-scFvs derived from Ofatumumab; a fully human mAb, differing in two widely used linkers. Our study generated two distinct scFvs; scFv-whitlow and scFv-G4S3 using protein modeling and post MD simulation analysis revealed that scFv-whitlow is more stable than scFv-G4S3 indicating that the linker impacts the scFv structure and orientation. Next, to investigate the binding mode with membrane bound CD20, molecular docking and MD simulations were performed. The scFv-whitlow complex demonstrated greater stability, less flexibility, a more stable interaction network with CD20 than the scFv-G4S3 complex. Binding energy calculations further confirmed a stronger binding affinity for scFv-whitlow & Per-residue energy decomposition revealed a greater number of actively interacting residues. These findings suggest the whitlow linker enhances scFv-CD20 complex stability and binding, thus it may be a more promising candidate for the development of anti-CD20 CAR-T cell therapies.

Keywords: CART, scFv, anti-CD20 CAR-T, Docking, Simulation.

P17 – Title: Hyaluronic Acid in Personalized Dermatology: Integrating Bioinformatics and Molecular Simulations

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Abstract:

Hyaluronic acid (HA) is a celebrated ingredient in modern skincare, known for its exceptional hydrating, anti-aging, and barrier-repair properties. Despite this widespread use, ranging from moisturisers and serums, to sunscreens and foundations, the efficacy of HA-based formulations varies significantly across different skin types, environmental conditions, and interactions with other skincare ingredients and common skin flora. This review investigates the mechanisms driving HA's functionality, focusing on its interactions with hyaluronic acid-binding proteins (HABPs), collagen, elastin, and proteoglycans under varying environmental and biochemical conditions and integrate their outcomes on skin health into a database. Building on these insights, this paper proposes a novel framework that integrates computational simulations, molecular docking, and basics of supervised learning within machine learning models to personalise HA-based skincare formulations. This project aims to predict the optimal conditions and formulations for individual skin profiles by simulating HA-protein binding across diverse scenarios and correlating the results with real-world data.

Keywords: Hyaluronic Acid, Molecular Docking and Simulations, Personalised Skincare

P18 - Title: Harnessing Bacteriophages to Combat Multidrug-Resistant *E. coli* in Wastewater Systems.

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Abstract:

Bacteriophages have recently piqued the interest of many in the fight against antibiotic-resistant bacteria. Wastewater treatment plants, due to antibiotic residues, microbial interactions, and gene transfer, serve as hotspots for multidrug-resistant (MDR) bacteria *E. coli*, particularly antibiotic-resistant strains, enter wastewater through human faeces and may spread resistance to the environment.

This study investigated the presence of MDR *E. coli* in the wastewater from 6 treatment plants distributed across Mumbai. Out of 106 strains identified during 12 months study period, 86 were found to be MDR. The seasonal variation in the prevalence of MDR *E. coli* was observed, with the highest occurrence in winter (47%), followed by summer (27.9%) and monsoon (24.4%), indicating potential environmental on bacterial persistence. Phages were successfully isolated against 46 out of the 86 MDR *E. coli* isolates. Final phage lysates were shortlisted based on their characteristics of being lytic, having broad host range, the resistance profile of the host and ability to grow to high titers in the lab. Thus, 4 *E. coli* lysates and the 5 MDR *E.coli* were selected and further studies for their Host reduction capacity. All four phage lysates were tested against five MDR *E. coli* hosts over six hours to assess reduction potential. A phage consortia approach was also evaluated, where a multiplicity of infection (MOI) of 1 reduced bacterial counts from log 8 to log 3, while an MOI of 10 led to complete eradication (log 8 to 0), demonstrating the superior efficacy of a higher phage dose. Future studies will focus on testing this phage consortium in a wastewater system and further characterization of these phages to assess their stability and efficacy. This approach holds promise for application in wastewater treatment, offering a sustainable biocontrol strategy for reducing MDR *E. coli* contamination.

P19 – Title: Exploring the efficacy and mechanism of action of multitarget inhibitor ONC2 01 in triple negative breast cancer

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Abstract: Triple-negative breast cancer (TNBC) is an aggressive subtype characterized by the absence of estrogen receptor, progesterone receptor, and HER2, making conventional endocrine and targeted therapies ineffective. Doxorubicin remains a cornerstone of TNBC treatment, but its clinical utility is limited by toxicity and resistance. ONC201, a novel imipridone currently in phase II trials, exhibits broad-spectrum anticancer activity via TRAIL pathway activation and mitochondrial ClpP hyperactivation. This study evaluates the cytotoxicity and mechanism of action of ONC201 in combination with doxorubicin in TNBC cell line (MDA-MB-231). Cytotoxicity assays identified synergistic drug combinations, with combination index (CI) values confirming synergy. Flow cytometry revealed that the combination induced significant G2/M phase arrest. Additionally, ONC201 downregulated doxorubicin-induced p21, a senescence marker, and Beclin-1, an autophagy marker, suggesting a potential role in overcoming doxorubicin-induced senescence. Recovery experiments further confirmed that ONC201 mitigates doxorubicin-induced senescence. These findings highlight ONC201 as a promising candidate for combination therapy to enhance TNBC treatment efficacy while mitigating chemotherapy-induced resistance.

Keywords: ONC201, triple negative breast cancer, doxorubicin, senescence, drug resistance

P20 – Title: Isolation and characterization of Lactic Acid Bacteria as probiotic from dairy and fermented food samples

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Abstract: Probiotics are live microorganisms that when administered in adequate amounts, confer health benefits on the host. LAB group can be isolated and characterized from dairy sources. This study aimed to isolate probiotics from dairy products and evaluate their potential probiotic properties, i.e. tolerance to acid, bile and gastric juice; auto-aggregation and co-aggregation ability. For this purpose, 21 different probiotics were isolated on the basis of their Gram nature and catalase activity from dairy products like Curd, Lassi, Idli batter, Jalebi batter ten samples of which from Mumbai were collected and screened. Acid, Bile and Pancreatin tolerance of 21 isolates were evaluated and 11 isolates showed significant tolerance to it which can be use as potential probiotic. Out of 21 isolates 11 isolates shown significant acid, bile and pancreatin tolerance ability and 14 showed time-dependent increase in auto-aggregation from 50% to 100% after 5 hours of incubation. Mixed consortia of isolates showed co-aggregative rate of 66.67%. 14 LAB isolates which were grown on Congo red MRS agar showed red colored colonies indicates the adhesion ability of bacteria. These findings highlight potential of these isolates to form protective clusters, aiding in their survival and colonization within the gastrointestinal tract, besides competitive exclusion of pathogens. These findings indicate that isolates can withstand harsh GI conditions, highlighting their suitability as probiotics. Overall, the result indicates that isolates from dairy and fermented samples used in this study exhibit potential probiotic traits. Further study can be done for their safety, efficacy and use in probiotic supplement.

Keywords: Probiotics, Acid tolerance, Auto-aggregation, Co-aggregation

P21 – Title : Exploring the Role of Natural Transformation in Nutrition and DNA Repair of Stressed *Deinococcus radiodurans*.

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Abstract: *Deinococcus radiodurans* stands out in the bacterial domain due to its exceptional resilience to ionizing radiation, desiccation, oxidative stress, and non-ionizing radiation (e.g., ultraviolet light). This organism possesses a highly efficient and precise DNA repair mechanism, alongside robust protein protection systems against oxidative damage. Contributing factors to its enhanced radiation resistance include a high guanine-cytosine (GC) content, a compact genome organization with histone-like proteins, a toroidal genomic architecture, and its characteristic tetrad structure. *D. radiodurans* utilizes an unconventional repair process, capable of resolving hundreds of double-strand breaks within hours, through two major pathways: RecA-independent Single-Strand Annealing (SSA) and RecA-dependent Extended Synthesis-Dependent Strand Annealing (ESDSA), essential for recovery after gamma radiation exposure. The organism also maintains natural competence throughout its growth cycle, with key components such as PilT, ComEA, ComEC, DprA, ComF, and RecA facilitating the uptake, protection, and incorporation of external DNA. Additionally, DprA plays a pivotal role in the differential regulation of DNA double-strand break (DSB) repair pathways, contributing to *D. radiodurans* survival under gamma radiation stress.

The first significant observation involves a differential survival response among mutants lacking specific NT-associated genes when exposed to gamma radiation and Mitomycin C (MMC). While the Δ*comEA* and Δ*pilT* mutants exhibited survival rates comparable to the wild type, the Δ*endA* and Δ*dprA* mutants demonstrated reduced survival under certain stress conditions. Notably, the Δ*endA* mutant exhibited increased sensitivity to gamma radiation and a marked decline in survival upon MMC exposure, suggesting the *endA* gene's potential role in mitigating MMC-induced DNA damage. Although growth patterns of these mutants under normal conditions resembled those of the wild type, deficiencies became apparent following gamma irradiation or MMC treatment, particularly in the Δ*endA* and Δd*prA* mutants, indicating impaired DNA repair mechanisms.

Keywords: Radioresistance, DNA repair, Nutrient, natural competence

P22 – Title: Biosynthetic Silver Nanoparticles from *Mussaenda philippica L.* for UTIs Biofilm Inhibition

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Abstract: Urinary Tract Infections (UTIs) are among the most prevalent infections, with *Klebsiella pneumoniae* and uropathogenic *Escherichia coli* (UPEC) as major causative agents. These pathogens form biofilms, enhancing their persistence and antibiotic resistance, challenging treatment. Targeting quorum sensing (QS) is an effective strategy to inhibit biofilm formation and associated virulence factors. This study reports, for the first time, the green synthesis of silver nanoparticles (AgNPs) using *Mussaenda philippica* L. leaf extract (Mp-AgNPs) and evaluates their antibiofilm potential against *K. pneumoniae* and UPEC. Clinical isolates were identified using MALDI-TOF and 16S rRNA sequencing. Mp-AgNPs were synthesized by optimizing plant extract concentration (1%), silver salt concentration (1.3 mM), reaction temperature (30 °C), and pH (9). The nanoparticles were characterized using UV-Vis spectroscopy, XRD, FT-IR, SEM, TEM, NTA, DLS, and zeta potential analysis. Antibiofilm efficacy was assessed using qualitative and quantitative assays, including the tube assay, Congo red assay (CRA), biofilm inhibition assay (BIA), and EPS quantification. Results demonstrated that Mp-AgNPs significantly reduced QS-mediated virulence factors, inhibiting biofilm formation by 56.67% in *K. pneumoniae* and 54.21% in UPEC, while exopolysaccharide production was reduced by 37.73% and 35.46%, respectively. These findings suggest that Mp-AgNPs can effectively disrupt QS and biofilms, making them a promising alternative to conventional antibiotics for managing biofilm-associated uropathogenic infections.

Keywords: Biofilm, *Mussaenda Philippica*, Quorum sensing, UPEC, Silver nanoparticles, Urinary Tract Infections.

P23 – Title: Anti-cancer Potential of Deuterium Depleted Water (DDW) on Human Cancer Cells is Linked to Altered Expression of Metabolic Target Regulators

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Abstract: Deuterium is a stable isotope of hydrogen, naturally present at high amount (~150 ppm) in natural water and plays a significant role in normal biological processes. Different strength of deuterium depleted water (DDW) has been used as an adjuvant for cancer patients in different parts of world. However, the underlying mechanisms is still not well established. Therefore, this study aims to estimate characteristic cellular and subcellular changes in breast and lung cancer cells when treated with lowered deuterium water.

Human cancer cell lines, MCF-7, ZR75-1, HCC1954 and A549 were adapted in culture media prepared with three different variant DDW water (32, 70, 110 ppm) along with control media condition (150 ppm) for five passages. Post-adaptation, survival and toxicity assays were performed which indicated a significantly lower cell survival in the 32 and 70 ppm DDW condition in comparison to 150 ppm, indicating an anti-proliferative effect in low deuterium water. Using electron microscope (TEM), we also saw a significant decrease in mitochondrial length in MCF-7 and A549 cells. Thereafter, live cell mitochondrial imaging was performed in aggressive breast cancer cell line HCC1954 and found the mitochondria morphological changes were associated with an increase in Mitochondrial membrane potential, reactive oxygen species (ROS) and Mitochondrial ROS in 32 and 70 ppm DDW adapted cancer cells. Enhanced cellular glucose uptake was found in 32 and 70 ppm adapted cells. We also performed AKT and MAPK kinase array to measure activated enzyme kinases that regulate numerous crucial cell functions. The array result showed increased amount of key activated kinases like AMPK, RSK1, RSK2 and PDK1 etc., hinting on major changes in metabolic control switches within cancer cell in low DDW condition potentiates lower proliferation.

These findings suggest that low DDW condition can downsize cancer cell growth and proliferation and such phenotypes may be linked to altered cellular and mitochondrial metabolism.

Keywords: Cancer cell; Deuterium depleted water; Mitochondria; Metabolism.

P24 – Title: Investigating the association of mutant p53-driven HER2 biology in Indian Gastric Cancer patients

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Introduction

Gastric cancer (GC) is primarily treated with surgery & cytotoxic chemotherapy (5-fluorouracil & platinum), but relapse is common. HER2 & VEGFR2-targeted agents offer limited response (10-40%). TCGA (2014) & ACRG (2015) suggest that 50% of GC have p53 mutations. In multiple cancers, mutant p53 regulates HER2 signaling. This study explores the p53–HER2 relationship in GC cell lines & Indian patients.

Material & **Methods**

IHC & NGS were performed in FFPE patient-derived tumor blocks. Wtp53 & patient-derived p53 mutation (R175H/R273H/L344N) were overexpressed in KATO-III$^{p53-/-}$ cells using site-directed mutagenesis. HER2 regulation by wtp53 and mutp53 was analyzed using immunoblotting and ChIP, while HER2 localization in mutp53-expressing cells was assessed by immunofluorescence.

Results & **Discussions**

In locally advanced Indian GC samples (n=32), pathogenic mutations were identified in TP53 (46%), NF1(31.3%), PTEN (21.9%), BRCA1 (18.8%), BRCA2 (18.8%). 51% of patients showed >70% expression/negative staining for p53 (both indicative of mutp53), as observed by IHC (n=47) & verified by NGS (n=32). Interestingly, 8.5% of patients showed high HER2 expression (Score 3+) by IHC & all harbored mutant p53. 4-fold & 3-fold upregulation of HER2 transcript & mRNA respectively, & enhanced membrane localization (vs wtp53) was observed in p53 mut-L344N KATO-III cells. ChiP assay revealed 6-fold increase in p53 binding on the HER2 promoter. ERK and AKT signaling were activated in p53 mut-L344N HER2-overexpressing cells.

Conclusion

Elucidating specific mechanisms of mutp53-mediated HER2 signaling would decipher the underlying molecular complexity of HER2 biology and its impact on diagnostic and therapeutic aspects for HER2-positive gastric cancer.

P25 – Title: Phosphoacetylation Mark in Gastric Cancer: Implications For Stress Conditions and Tumor Progression

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Background: Histone post-translational modifications (PTMs) regulate gene expression and contribute to disease progression, including cancer. In gastric cancer, elevated H3S10 phosphorylation (H3S10ph), driven by the p38-MSK1 pathway, associates with poor prognosis. When coupled with H3K14 acetylation (H3S10phK14ac), this dual modification drives transcriptional activation, influencing oncogenes such as *c-fos* and *c-jun*. However, its functional significance in cancer remains unclear.

Objective: To investigate the role of H3S10phK14ac in transcriptional regulation under stress and during early gastric tumorigenesis in an animal model.

Methods: Gastric cancer cells were subjected to serum starvation and hypoxia, followed by histone isolation and PTM analysis. RNA sequencing (RNA-seq) was performed to assess transcriptional changes. A gastric cancer model was established in C57BL/6 mice using methyl-nitrosourea (MNU) and salt. Immunohistochemistry was used to evaluate histone modifications in tissues.

Results: H3S10phK14ac levels exhibited a marked decline under stress conditions. Transcriptomic analysis demonstrated a downregulation of genes involved in metabolic and signaling pathways. Additionally, key chromatin modifiers essential for the establishment of the phosphoacetylation mark, such as MSK2 and Gcn5, were also found to be downregulated. Cells deprived of growth factors showed reduced expression of cyclins, cyclin-dependent kinases (CDKs), elongation factors, and histones. In the in-vivo model, early tumorigenic alterations, including hyperplasia and dysplasia, were observed. Immunohistochemical analysis further validated significant changes in H3S10ph, H3K14ac, and H3S10phK14ac levels in early-stage gastric tumors.

Conclusion: The significant alteration of H3S10phK14ac, along with significant gene expression changes, suggests its involvement in stress adaptation and early cancer progression. Understanding its genomic association could provide insights into gastric cancer pathogenesis and potential therapeutic strategies.

Key words: Gastric cancer, histone post translation modification, epigenetics, stress response

P26 – Title: The Surprising Effects of Zinc Stress: Silencing Chromatin by Compaction

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Abstract: Environmental stress drives gene silencing in mammals through a collaboration of three epigenetic pathways, i.e., DNA methylation, Polycomb methylation (PcG), and histone deacetylation (HDACs). To assay for conserved mechanisms that can track heritable changes in gene silencing, we used *Chlamydomonas,* a volvocene chlorophyte that harbours these three pathways. A Paromomycin resistance ($Paro^R$) transgene was randomly integrated to populate a library of transgenic clones. The *Epigenetic assay* was used to track position-effect variegation in these libraries, by measuring a quantitative loss of antibiotic resistance in populations (due to silencing), uncovering Cu and Zn stress-induced silencing. While oxidative stress (ROS) emerged as the causal mechanism for Cu, the basis of Zn-stress induced silencing remained unexplored. Transcript analysis (by qPCR) and zymograms indicated a reduction in mRNA levels and concomitant protein, indicative of endogenous genes getting affected by Zn stress. A dose dependent exposure revealed a spike of intracellular Zn at 110 µM (normal concentration: 76 µM) as corroborated by both ICP-MS measurements and nuclear staining of free Zn by Fluozin-3 AM. Quantitative measurements using propidium iodide revealed a concomitant decrease in nuclear size as a function of Zn dose. Molecular epigenetic analyses using Micrococcal Nuclease revealed an increase in the average nucleosomal length, a feature typical of compacted chromatin in differentiated cells and gametes. In conclusion, we propose that Zn stress leads to accumulation of free Zn that induces chromatin compaction. This study opens the door to querying effects of Zn stress in eukaryotes revealing a hitherto undescribed epigenetic mechanism of adaptation to Zn, one of the most tolerated and widely used metal supplements in disease and immune therapy.

Keywords: gene silencing, chromatin compaction, nucleosomes, intracellular zinc.

P27 - Title: Evaluating the Compatibility and Antagonistic Activity of *Pseudomonas putida* and Endophytic *Lactobacillus plantarum* Isolates for the Biocontrol of Soybean Leaf Blight Caused by *Xanthomonas campestris* pv. *glycines*

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In this study, we evaluated the biocontrol potential of endophytic *Lactobacillus plantarum* and rhizosphere-derived *Pseudomonas putida* against *Xanthomonas campestris* pv. *glycines*, the pathogen isolated from soybean leaf blight. Ten isolates of *L. plantarum* (designated LP1–LP10) were obtained from fermented cabbage, while *P. putida* was isolated from the rhizosphere of healthy soybean plants. Initially, to ensure that both beneficial bacteria could coexist, we performed a compatibility test by spotting *P. putida* onto a growing lawn of *L. plantarum* culture. Out of the ten isolates, LP-1, LP-2, LP-5, and LP-6 were found to be compatible with *P. putida*, whereas the remaining isolates produced a clear zone of inhibition. These four compatible isolates were then selected for further investigation. Following confirmation of mutual growth compatibility, antagonistic activity against *X. campestris* pv. *glycines* was assessed using the streak method (Raja et al., 2016).

Results indicated that *P. putida* exhibited marked antagonistic activity against the pathogen, whereas none of the *L. plantarum* isolates showed direct inhibition. The pathogen was isolated from symptomatic soybean leaves using Yeast Extract Glucose Calcium Carbonate agar (YGCA). In addition, a bacteriocin was isolated from *P. putida* cultured in Tryptic Soy Broth (TSB) and was assayed using the agar cup method, revealing a significant zone of inhibition against *X. campestris*. These findings underscore the potential of *P. putida* and its bacteriocin as natural biocontrol agents for managing soybean leaf blight. Future studies will focus on optimizing bacteriocin production and evaluating field-level efficacy to develop integrated disease management strategies.
