MIT School of Bioengineering Sciences & Research

(A constituent unit of MIT ADT University, Pune, India)

6th INTERNATIONAL CONFERENCE

ON

RECENT TRENDS IN BIOENGINEERING

(ICRTB 2023)

Friday, January 20 & Saturday, January 21, 2023

ABSTRACTS




MIT School of Bioengineering Sciences & Research
Pune

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Bioengineering Sciences & Research
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About ICRTB 2023

International Conference on Recent trends in Bioengineering (ICRTB) is an annual flagship event, organized by MIT School of Bioengineering Sciences & Research, Pune. The main objective is to bring together engineers, researchers and practicing clinicians, academicians and those working in the industry luminaries and government agencies to discuss the latest research in bioengineering and allied fields. Bioengineering is a novel and multi disciplinary field which works towards bridging the gap between engineering and biology. It has gained immense importance in the global market. This is a unique conference that would bring together engineers, clinicians, industry and academia to find bioengineering solutions in health care and environment.

Conference Theme Areas

Conference Theme : Bioengineering Solutions for Health and Environment

Sub Themes :

- Biosensors
- Drug delivery systems
- Biomaterial for clinical diagnostics
- Environment Monitoring
- Bio-inspired materials
- Medical Robotics
- Biomaterials
- Biofertilizers and Biopesticides
- Biomedical imaging
- Bioremediation
- Medical wearable devices and Diagnostics
- Bioinformatics

6th International Conference on Recent Trends in Bioengineering (ICRTB-2023)

Editors
Prof. Vinayak Ghaisas
Dr. Renu Vyas

Organized by

MIT School of Bioengineering Sciences & Research
MIT, Art, Design and Technology University, Pune-412201, India

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6th International Conference on Recent Trends in Bioengineering (ICRTB–2023)

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Dedicated to
in loving memory of

Late Hon'ble Dr. Suresh Ghaisas

A great doctor and a greater human being!!
Your life was a blessing. Your memory a treasure.
You shall always stay with us.

Messages

Hon. Prof. Dr. Vishwanath Karad

My deep appreciation and congratulations to MIT School of Bioengineering Sciences & Research, a constituent unit of MIT Art, Design and Technology University Pune for its annual flagship event- the 6th International Conference on Recent Trends in Bioengineering (ICRTB 2023).
It gladdens my heart to note that the institute has achieved great heights in a very short span of time. I convey my blessings to tomorrow's innovative knowledge leaders and budding talent of delegates.

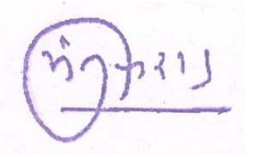
Prof. (Dr.) Vishwanath D. Karad
Founder MIT Group of Institutions
President, MIT Arts, Design & Technology University, Pune

Dr. Mangesh Karad

Dear Delegates

I am very happy to note that MIT School of Bioengineering Sciences & Research is organizing the 6th International Conference on Recent Trends in Bioengineering (ICRTB 2023). Every such event fuels growth for innovation and research at Institute, University and academia at large. The deliberations of ICRTB will serve to activate curiosity, knowledge and new vision into the frontier areas of Bioengineering. It is heart-warming to see one of our institute prioritizing next generation by organizing this outstanding and insight-full conference on relevant topics with deep impact on society.

With such endeavours, MIT Arts, Design & Technology University is poised to become one of the leaders in providing good research output and strengthening the research innovation ecosystem.



Hon. Dr. Mangesh Karad
Executive President & Vice-Chancellor
MIT-ADT University

Prof. Vinayak Ghaisas

I am very happy that every year we are effectively conducting our International Conference on Recent Trends in Bioengineering (ICRTB) and improving the collective knowledge in the field of Bioengineering. Over the past years the conference is receiving very good response across the nation. Speakers from India and abroad having valuable experience have been drawn across multiple disciplines. I am sure that delegates will get exposed to new ideas and learn tremendously from these talks. The theme of the conference is Bioengineering solutions for healthcare and environment. Bioengineering is a niche field that has immense potential to provide sustainable solutions for the betterment of society.

Warm welcome to all delegates, speakers and hope you enjoy our hospitality.

Prof Vinayak Ghaisas
Founder Director
MIT School of Bioengineering Sciences & Research
Managing Trustee, MAEER Pune
Convenor ICRTB 2023

Dr. Renu Vyas

With deep sense of satisfaction and pride in the growth of the institute, I welcome all the delegates, guests and speakers from research, academia and industry to the 6th International Conference on Recent trends in Bioengineering (ICRTB 2023). The quality of abstracts and the geographical diversity of registered participants is enhancing every year along with the profile of the speakers.

ICRTB is a wonderful platform that focuses not only on research components of frontier areas of research but also on industry influenced solutions and innovations. This philosophy and culture of cross functional collaboration is rare in India and it is wonderful to see it coming together on a single platform.

We hope to continue our unrelenting efforts and passion with each passing year.

Looking forward to meeting everyone.

Dr. Renu Vyas

Head of the School
MIT School of Bioengineering Sciences & Research
Dean, Faculty of Technology, MIT ADT University, Pune
Convenor ICRTB 2023

Eminent Speakers

Prof. Pawan K. Dhar

Professor, School of Biotechnology, Jawaharlal Nehru University, New Delhi

Profile

Professor Pawan K. Dhar heads Synthetic Biology group at the School of Biotechnology, Jawaharlal Nehru University, New Delhi. He is also the CoFounder of Foresight Biotech Pvt. Ltd. (focus: drug discovery) and ClearMeat Pvt. Ltd. (focus: lab grown meat). In 2007, Prof. Dhar established the Systems and Synthetic Biology Journal, Springer with Prof. Ron Weiss (MIT) and ran it for nine years. Some of his significant contributions have been (a) developing ClearX9 - a slaughter free, effective, and affordable alternative to the Fetal Bovine Serum (b) making functional genes and proteins from the dark matter of genome (c) developing synthetic biology governance framework for Government of India. In the past, Prof. Dhar has established research groups in India, Singapore, and Japan and published in the areas of human genetics, systems biology, and synthetic biology covering computational, experimental, and policy areas.

Talk synopsis

THE DARK GENOME

Prof. Pawan K. Dhar

Abstract : From the functional standpoint, three kinds of DNA sequences exist: one that encode proteins, second that encode only RNA (non-coding DNA) and third that do not transcribe (non expressing DNA). Historically people have paid attention to the protein coding genes. For the last two and a half decades, the non-coding RNA has taken the center stage in biology. However, the non-expressing (dark) genome is a relatively unexplored space. We asked: How

did nature decide to allocate protein coding and RNA coding jobs to a specific set of sequences? Given a large sequence space between the genes, did she sample all possibilities, retaining good results (protein and RNA encoding genes), retiring not-so-relevant results (pseudogenes), leaving some DNA sequences unattended (non expressing genome). To answer these questions, we developed a novel approach for designing synthetic genes and demonstrated their expression and phenotypic outcomes. The success of this initial experiment emboldened us to look for naturally non-expressing regions which, when artificially expressed, could make user defined proteins towards functional endpoints. In my talk, I shall describe our journey in a less explored space of dark genome, provide computational and experimental evidence towards emergence of what we would like to call - Functional Genomics 2.0.

Prof. Jeremy C. Simpson
Full Professor of Cell Biology
School of Biology & Environmental Science
University College Dublin (UCD)
Dublin, Ireland

Email: jeremy.simpson@ucd.ie
Tel: +353 (0)1 716 2345

Profile

Jeremy Simpson obtained his PhD from the University of Warwick (UK). After post-doctoral work at the Scripps Research Institute (San Diego, USA) and the ICRF (London, UK), a long term EMBO fellowship took him to the EMBL (Heidelberg, Germany), where he developed and applied novel high-throughput imaging approaches to study protein localisation and membrane traffic in mammalian cells. In 2008 he was appointed as Full Professor of Cell Biology at University College Dublin (Dublin, Ireland). His lab applies high-throughput imaging technologies to study intracellular trafficking pathways, diseases associated with the endomembrane system of cells, and the internalisation routes taken by synthetic nanoparticles as drug delivery vehicles. His lab also develops novel 3D cell models allowing the quantitative study of cell behaviour at multiple scales. He has authored 125 peer-reviewed articles, including articles in Nature Cell Biology, Nature Communications, Nature Methods and Scientific Reports and runs the UCD Cell Screening Laboratory (www.ucd.ie/hcs). He is currently also serving as the College Principal and Dean of Science in the UCD College of Science.

Talk synopsis

Genome-wide RNAi screening combined with high content imaging to understand how nanomaterials interact with mammalian cells

Prof. Jeremy C. Simpson

Nanomaterials present great potential for precise and controlled delivery of therapeutics to specific tissues and organs. However, despite the massive interest in their development, we know relatively little at the molecular level in terms of how they interact with cells, how they are internalised, and the cellular responses that they invoke.

We are using a combination of genome-wide RNA interference and automated high content screening microscopy to systematically dissect the mechanisms by which fluorescently-labelled synthetic nanoparticles interact with cells and then enter them [1]. Our screens for the first time reveal key cellular proteins that play a role in their trafficking, allowing us to more precisely identify the membrane compartments that they come into contact with [2,3]. We also employ a range of both 2D and 3D model cell systems, which are helping us evaluate potential limitations of using nanomaterials in complex cellular environments.

The information that we gather provides a deeper systems-level view of how cells are organised, and provides knowledge fundamental to the design of next generation drug delivery vectors and biomedical devices.

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Dr. Mohan Wani
Director,
National Centre for Cell Science, Pune

Profile:

Dr. Mohan Wani is working as Director and Scientist G (Professor) at National Centre for Cell Science, Pune, India. Dr. Wani did his Masters degree in Veterinary Surgery from Nagpur Veterinary College and PhD in Medicine from St. George's Hospital Medical School, University of London, England. He was awarded with a prestigious “Commonwealth Fellowship” during his PhD. He has made innovative basic and translational research in the field of “Pathophysiology of bone and cartilage remodeling in important skeletal diseases such as osteoporosis, rheumatoid arthritis and osteoarthritis”. He also has expertise in stem cell science and regenerative medicine. Dr. Wani has supervised several PhDs, medical/dental and veterinary students and mentored many postdoctoral fellows. His research work is published in several reputed international journals and patents. He is recipient of several prestigious awards including Commonwealth Fellowship, B. M. Birla Science Prize, DBT National Bioscience Award, Tata Innovation Fellowship, Fellow of National Academy of Sciences (FNASc) and Indian National Science Academy (FNA).

Justin Dauwels
Associate Professor, TU Delft

Profile

Dr. Justin Dauwels is an Associate Professor at the TU Delft (Circuits and Systems, Department of Microelectronics). He was an Associate Professor of the School of Electrical and Electronic Engineering at the Nanyang Technological University (NTU) in Singapore till the end of 2020. He was the Deputy Director of the ST Engineering – NTU corporate lab, which comprises 100+ PhD students, research staff and engineers, developing novel autonomous systems for airport operations and transportation.

His research interests are in data analytics with applications to intelligent transportation systems, autonomous systems, and analysis of human behaviour and physiology. He obtained his PhD degree in electrical engineering at the Swiss Polytechnical Institute of Technology (ETH) in Zurich in December 2005. Moreover, he was a postdoctoral fellow at the RIKEN Brain Science Institute (2006-2007) and a research scientist at the Massachusetts Institute of Technology (2008-2010). He has been a JSPS postdoctoral fellow (2007), a BAEF fellow (2008), a Henri-Benedictus Fellow of the King Baudouin Foundation (2008), and a JSPS invited fellow (2010, 2011).

He served as Chairman of the IEEE CIS Chapter in Singapore from 2018 to 2020, and serves as Associate Editor of the IEEE Transactions on Signal Processing (since 2018), Associate Editor of the Elsevier journal Signal Processing (since 2021), member of the Editorial Advisory Board of the International Journal of Neural Systems, and organizer of IEEE conferences and special sessions. He is also Elected Member of the IEEE Signal Processing Theory and Methods Technical Committee and IEEE Biomedical Signal Processing Technical Committee, both since 2018.

His research on intelligent transportation systems has been featured by the BBC, Straits Times, Lianhe Zaobao, Channel 5, and numerous technology websites. Besides his academic efforts, the team of Dr. Justin Dauwels also collaborates intensely with local start-ups, SMEs, and agencies, in addition to MNCs, in the field of data-driven transportation, logistics, and medical data analytics.

Talk synopsis

AI for applications in psychiatry

Justin Dauwels
Associate Professor, TU Delft

Abstract:
Many tasks in medicine still involve substantial manual work. In many cases there is strong potential for intelligent automation by A.I., leading possibly to a reduction in costs and man-hours, while increasing the quality of clinical service. In this talk, we will consider applications of A.I. in the domain of psychiatry.
Specifically, we will give an overview of our research towards automated behavioral analysis for assessing the negative symptoms of mentally ill patients.

Gagandeep Kang

Professor, Division of Gastrointestinal Sciences, Christian Medical College. Vellore, India

Profile:

Professor Kang is a physician scientist working on vaccines and public health, particularly focused on children and enteric infectious disease in India. She has worked with colleagues at the Christian Medical College (CMC) and others institutions in India to build national rotavirus and typhoid surveillance networks to estimate disease burden, test vaccines and inform policy. Based at CMC for most of her career, she has established strong training programmes for students and young faculty in clinical translational medicine and public health aiming to build a cadre of clinical researchers studying relevant problems in India.

Dr. Natalie Artzi

Principal Research Scientist,MIT Institute of Medical Engineering & Science,Cambridge, Massachusetts, USA

Profile:

Dr. Artzi is an Assistant Professor at the Department of Medicine, Division of Engineering in Medicine, Brigham and Women's Hospital, Harvard medical School. She is a Principal Research Scientist at MIT and an Associate Member of the Broad Institute of Harvard and MIT. She completed her postdoctoral studies at the laboratory of Prof. Elazer Edelman at MIT focusing on studying tissue:biomaterial interactions and designing smart biomaterials for therapy and diagnosis applications. Dr. Artzi is the recipient of multiple grants and awards, including the One Brave Idea award, Stepping Strong Innovator Award, Controlled Release Society Young Investigator Award, Mid-Career Award from the Society for Biomaterials, Bright Futures Prize, and the Massachusetts Life Science Center for women entrepreneurs. Currently, Dr. Artzi directs multiple research venues aiming to integrate science, engineering and medicine to rationally design personalized materials to improve human health, and has co-founded a startup company, BioDevek, which develops the next-generation biomaterials to improve outcomes following internal surgeries.

Talk synopsis

Engineering therapeutic immunity to glioblastoma through the intracranial delivery of chemoimmunotherapy using adhesive hydrogels

Authors: Michelle Z. Dion, Safwan Alomari, Pere Dosta, Daniel Dahis, Alex Cryer, Núria Puigmal, Ivana Ling, Betty Tyler, Henry Brem, Natalie Artzi

Immunotherapy is a promising modality for the treatment of glioblastoma (GBM) due to its ability to stimulate specific, potent anti-tumor immune

responses; however, like in many other solid tumors, only a subset of patients has derived clinical benefit. This lack of efficacy can be partially attributed to the inability of immunomodulatory agents to achieve the appropriate spatiotemporal kinetics to elicit therapeutic responses when administered systemically, and due to the inability of monotherapy to overcome the numerous immunosuppressive mechanisms and rapid growth rate of GBM. In this study, we investigated the efficacy and immunomodulatory mechanisms of local hydrogel-mediated delivery of chemoimmunotherapy—a cyclic dinucleotide (CDN) stimulator of interferon gene (STING)-agonist and doxorubicin—in combination with checkpoint blockade antibodies. STING agonists are powerful immunomodulatory therapeutics as they induce the production of Type I interferons and other proinflammatory cytokines, which enhance the recruitment and activation of dendritic cells that can license both T-cell dependent and independent (natural killer cell, macrophage) anti-tumor immunity. We hypothesized that the local delivery of combination CDN and doxorubicin chemoimmunotherapy using an injectable adhesive hydrogel would improve therapeutic outcomes by enabling efficient penetration and retention of chemoimmunotherapy in the tumor. This therapy will drive immunogenic cancer-cell death and the release of tumor antigens while potently activating immune cells in the tumor microenvironment and draining lymph nodes to propagate multi-axis tumor-specific immune responses and establish immune memory. In mice bearing orthotopic, syngeneic GL261 tumors, treatment with a single injection of chemoimmunotherapy hydrogel combined with systemic anti-PD-1 resulted in curative survival and potent immune memory protection from contralateral hemisphere rechallenge in all treated mice, whereas intratumoral injection of free therapies did not extend mouse survival. Pharmacokinetic and immunophenotyping studies demonstrated that local hydrogel therapy persisted for up to three weeks in vivo and induced significant alterations in multiple immune compartments of the tumor microenvironment and draining lymph nodes. Our results demonstrate that sustained local delivery of immunogenic therapies using our adhesive hydrogel platform can induce and maintain effective, durable immune responses that potently eliminate intracranial tumors and prevent their recurrence, establishing an effective platform for GBM immunotherapy.

Dr. Andreas Bender
Director of Digital Life Sciences at Innovation Campus Berlin (ICB)/Nuvisan Berlin.

Profile

Dr Andreas Bender is a Professor for Molecular Informatics at Cambridge University, working on data analysis methods related to compound safety and efficacy. Previously he was a Director for Digitial Life Sciences at Nuvisan in Berlin, as well as as an Associate Director for Data Science and AI in the Clinical Pharmacology & Safety Sciences group at AstraZeneca. On the entrepreneurial side, Andreas was involved in setting up Healx Ltd. (for data-driven drug repurposing) and PharmEnable Ltd. (for designing novel chemistry for targets that are difficult to drug conventially), both based in Cambridge/UK. He received his PhD from the University of Cambridge and worked in the Lead Discovery Informatics group at Novartis in Cambridge/MA as well as at Leiden University in the Netherlands as well as AstraZeneca before his current post.

Using Artificial Intelligence and Chemical and Biological Data for Drug Discovery: Opportunities and Pitfalls

While Artificial Intelligence (AI) had a profound impact on areas such as image and speech recognition, comparable advances in drug discovery are rare. In this contribution, we will firstly discuss in which ways chemical and biological data differs fundamentally from data available in other domains, both in its quantity and its underlying characteristics. Subsequently, case studies will be presented where the use of chemical and biological data, in combination with computational algorithms, has been successfully applied to questions related to compound mode of action, efficacy and safety. We will conclude by outlining what is needed in the future in order to advance the application of algorithms in the drug discovery field further, in particular with respect to the *in vivo* relevance of any predictions that are being made.

Ms. Kirsten Sinclair Rosselot
Director, Process Profiles,
California, USA

Profile

Kirsten Rosselot specializes in analyses for understanding and improving environmental performance. She taught an upper division/graduate student elective on pollution prevention in the chemical engineering department at California State University, Long Beach for two years and has co-authored many handbooks, textbooks, and other teaching and outreach materials, along with peer-reviewed literature.

Talk synopsis

Sustainable Bioengineering and Systems Thinking

Bioengineering solutions have the potential to improve the sustainability of many human activities, including food production, chemical and materials manufacture, and packaging. But how do you know if a new product or process is sustainable? It is not enough to consider only the emissions and waste streams from a process or the impacts at the end of life of a product. The system that is involved is larger than that. Ms. Rosselot will talk about applying systems thinking when determining sustainability and deciding where to draw the boundaries of the system and what to include in the system envelope.

Rahul Sharad Bhambure, PhD
Senior Scientist,
Chemical Engineering and Process Development Department,
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Profile

Dr. Rahul Bhambure leads the Bioprocess Technology group in Chemical Engineering and Process Development Division of CSIR-National Chemical Laboratory, Pune. His area of research covers both experimental and theoretical grounds applied mainly to the field of process and product development for biopharmaceuticals. For the last ten years, He has been working in the area of bioprocess development for recombinant protein and nucleic acid therapeutics. His future research interest is more focused on applied protein biophysics and biochemical engineering for developing novel processes at various stages of biopharmaceutical manufacturing like upstream, downstream and formulation.

Talk synopsis

Mapping covalent and non-covalent interactions during in-vitro refolding of therapeutic antibody fragments.

In-vitro refolding is the major rate-limiting step in the large scale manufacturing of recombinant antibody fragments expressed using microbial host cells. Understanding the effect of various parameters on protein refolding rates is a challenging task. In this investigation, covalent and non-covalent interactions during in-vitro refolding of antibody fragments were studied using multiple

orthogonal analytical techniques like circular dichroism, fluorescence and mass spectroscopic methods. Two model antibody fragments (Biosimilar rHu Ranibizumab and rHu Certolizumab) were expressed as inclusion bodies using E. coli host. Dilution based refolding process was optimized for in-vitro refolding of the antibody fragments from inclusion bodies. Refolding kinetics was analyzed using a three-parameter kinetic model. Time-dependent non-covalent interactions during in-vitro refolding were studied using fluorescence and circular dichroism spectroscopy whereas, time-dependent disulfide bond formation in antibody fragments was mapped using the liquid chromatography-tandem mass spectrometry (LC-MS/MS) based approach. Both collision-induced fragmentation (CID) and electron-transfer dissociation (ETD) based fragmentation was used to orthogonally map the disulfide bonds using high resolution and high definition mass spectroscopy. It was observed that inter-chain disulfide bond formation is the key rate limiting step in the overall refolding of the antibody fragments. Disulfide bond mapping shows that intra-chain disulfide bond formation in light and heavy chain of an antibody fragment is completed within 24 hours. In contrast, inter-chain disulfide bond formation requires about 48 hours, limiting overall process throughput. We conclude that compared to non-covalent interactions, covalent interactions majorly drive the in-vitro refolding rates of antibody fragments. We also conclude that ETD can provide significant alternative fragmentation information that complements CID-derived data to improve the disulfide bond mapping during in-vitro refolding of multi-domain proteins like antibody fragments.

Reza Abbasi-Asl, PhD

Assistant Professor, Neurology, Bioengineering and Therapeutic Sciences, UCSF
Director, Data Analytics and Visualization, Weill Institute for Neurosciences
Faculty, Neuroscape
Weill Neurohub Investigator
UC Berkeley, UCSF Bioengineering & UCSF Bioinformatics Graduate Programs
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Profile:

Dr. Reza Abbasi-Asl is an Assistant Professor in the Department of Neurology and the Department of Bioengineering and Therapeutic Sciences at UCSF and a core member at UCSF Neuroscape labs. He is a Weill Neurohub Investigator and serves as the director of Data Analytics and Visualization at the Weill Institute for Neurosciences at UCSF. He received his PhD and MSc in Electrical Engineering and Computer Sciences at UC Berkeley in 2018. His research lab investigates the role of interpretable machine learning in understanding brain functions and its related disorders. His research is supported through one RF1 award from NIH/NIMH, two Weill Neurohub awards, two Sandler Program for Breakthrough Biomedical Research awards, and one NIH R03 subaward. Dr. Abbasi-Asl is the recipient of the Eli Jury Award from UC Berkeley, Department of Electrical Engineering and Computer Sciences in 2018, the May J. Koshland Fund in Memory of H.A. Jastro Award from UC Berkeley Graduate Division in 2016, the Excellence Award in Biomedical Engineering from Sharif University of Technology in 2013, and the Excellence Award in Electrical Engineering from Tehran Polytechnic in 2010.

Talk synopsis

Spatio-temporal modeling in neuroscience through interpretable machine learning

In the past decade, research in machine learning has been exceedingly focused on the development of models with remarkably high predictive capabilities for both spatial and temporal datasets. Specifically, models based on deep learning principles have shown promise within domains such as neuroscience and healthcare. However, the non-linearity and the huge number of parameters in these models have made them difficult to interpret for domain experts. In this talk, I will discuss the importance of interpretable machine learning for scientific discovery in the context of multiple computational basic and clinical neuroscience studies with a focus on spatial and temporal datasets.

Prof. Sangeeta Kale
Professor in Physics & Director (Policy & Planning)
Defence Institute of Advanced Technology (DIAT), Pune
Co-Director, Navyukti Innovations Private Ltd., Pune
Contact: email: *sangeetakale2004@gmail.com* / *sangeetakale@diat.ac.in*

Profile

Sangeeta Kale, graduated from University of Pune, India and did her Masters in Electronic-Science and Doctoral studies in Material Science from same university. She did her post-doctoral studies from University of Maryland, College Park, U.S.A. She is working at Defence Institute of Advanced Technology, as Professor and Director (Policy & Planning) of this University. Additionally, she worked as a visiting Scientist at International Centre for Theoretical Physics (2006 – 2020), at Trieste, Italy. She co-owns a start-up company, "Navyukti Innovations Private Limited", where she works as the Director. Earlier, she worked as Officiating Vice Chancellor (2014-15) of DIAT and Dean (Academics) (2013-15, 2018-20), Dean (Student Affairs) (2017-18) of DIAT. At the research front, she works on nanomaterials for their sensing and biomedical applications, typically pertaining to Defence research (DRDO and Tri-Services (Army-Navy-Air Force)). She has successfully executed projects funded nationally from DST, DBT, UGC, DAE, ISRO and DRDO. She has guided more than 17 PhD students for their PhD and more than 50 Masters projects for their dissertations. She has more than 115 International research publications to her credit along with 8 Book Chapters and 4 Books. She has written a invited-chapter in a book entitled "Lilavati's Daughters" published by Indian Academy of Sciences, which is a short biography of Indian Women Scientists.

Talk synopsis

COMBINATION OF ENGINEERED RESONATORS AND NANOMATERIALS FOR SENSING HAZARDOUS ENVIRONMENTS

Prof. Sangeeta Kale

Sangeeta Kale*, Rajat Srivastava, Vivek Kale

Department of Applied Physics, Defence Institute of Advanced Technology (DIAT), Pune, INDIA
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Sensors based on Metamaterials (MMs)-based structures are becoming increasingly popular due to their benefits like high sensitivity, high-quality factor, label-free detection, and real-time measurements. These are engineered resonators which show excellent sensing capabilities, such as chemical sensing, gas sensing, and biological sensing.

This talk summarizes multiple efforts done by our group on the development of chemical sensors for hazardous environment detections (especially biological warfare agents) and disease-causing viruses. We have used resonator devices, in the form of complementary split-ring resonators (CSRR), which were tuned to ~430 MHz. The hazardous gases were subjected to various nanoparticles, depending upon their sensitivity towards specific molecular moieties, and the sensing was made more selective, and sensitive with the extremely low response and recovery times. Fe_3O_4 nanoparticles and Titanium dioxide (TiO_2) NPs are discussed for sensing hazardous NO_2 and SO_2 gases, respectively. A change in the resonant frequency and output power was measured as a function of ppm gas concentrations. The sensor showed excellent sensitivity and selectivity. Detailed chemical analysis which justifies the exclusive selectivity towards these hazardous biological moieties will be discussed in this presentation.

Keywords: Resonators; Sensor; hazardous molecules; dielectric constant; nanoparticles;

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Dr. Taslimarif Saiyed
CEO and Director, C□CAMP

Proifile:

Dr. Taslimarif Saiyed is the CEO and Director of C□CAMP from 2009 till present. His initial training has been in neurosciences, where he received his PhD from Max□Planck Institute for Brain Research, Germany from 2002□2006 and followed it up by postdoctoral training at University of California San Francisco (UCSF) from 2006□2009. At the same time, he also underwent training in management for Biotech and Innovation from QB3 at UC Santa Cruz, UC Berkeley and UC San Francisco from 2007□2009. He has also completed a biotech management program for biotech executives at Wharton School of Management in the year 2012. In the Bay area, he served as a Management Consultant with QB3 New BiotechVenture Consulting and in an individual capacity, he also consulted for many biotech firms inthe US.

Dr. Saiyed is an Adjunct Faculty at Indian Institute of Technology (IIT) Madras and also Amrita Institute □ School of Biotechnology since 2015. He also heads the Discovery to Innovation Accelerator program at C-CAMP. He is actively involved in promoting innovation in lifescience / healthcare by supporting translation of discoveries to application, entrepreneurship and technology development.

Dr. Jitendra Sharma

Managing Director & Founder CEO

Andhra Pradesh MedTech Zone (AMTZ)

Profile:

Dr. Jitendra Sharma is the Managing Director & Founder CEO of Andhra Pradesh MedTech Zone (AMTZ) which is World's first medical devices research and manufacturing park. He is Founder Executive Director of Kalam Institute of Health Technology (KIHT) – that serves as medical technology policy institute to various departments & ministries of Govt. of India. He is Member Secretary of National Medical Devices Promotion Council, and founder Chairman of two med-tech incubators – Medi-Valley, and Bio-Valley. He is adjunct lecturer at University of Adelaide, Australia; Chairman of Indian Biomedical Skill Council and a Distinguished Senior Fellow at Niti Aayog, the national policy making institution of Govt. of India. He has served as chairperson of several task forces on behalf of Govt. of India.

Dr Sharma has been awarded the European Union–India Young Leaders Award at EU Parliament, Brussels; Prestigious AAMI-Laufman Greatbatch Award and American College of Clinical Engineering Excellence Award for his distinguished work in medical technology sector. He has three academic doctorates and is author of book- "Made in Lockdown".

Atul Kurani
Vice president and head,
Medical and IoT business, Capgemini

Profile:

With over 32+ years of experience, Atul has been instrumental in building significant business in Product Engineering space. He leads global Medical Device in Capgemini Engineering. He also leads IoT / IIoT CoE and has built strong IoT solutions across Industry verticals. He has been part of product engineering services business since last 26 years and has worked across Industry sectors (Medical Devices, CPRD, Storage, Automotive, Industrial automation and Enterprise Software Product companies – ISVs) delivering innovative products and services. He is passionate technocrat and has led various COEs (Opensource, Cloud, Mobile, SaaS, etc) that become the practice with substantial business. He has also built key alliances with PTC, Microsoft (Azure), IBM and Software AG on IOT, AI, ML and on Immersive technologies. Atul has extensive international experience (14 years+ in North America, Europe & Asia-Pac and worked out of 42+ Countries) and is extremely good with building long term customer relationships using his technical expertise.

Talk synopsis

Connected Medical products are going to change the healthcare forever. India will lead the digital revolution and will contribute in improving healthcare at scale and at right price points. As a technocrats of future and with Passion to serve the mankind, Indian Engineering community will be in forefront in bringing this massive shift. Let us prepare and hone our skills to be “Innovators” with connected health opportunity. Welcome to world of IoMT (Internet of Medical things) that should make healthcare accessible and affordable for all.

Brig (Dr) Kannan Venkatnarayan
Officer on Special Duty,
NITI Aayog, New Delhi

Profile:

Is an alumnus of Armed Forces Medical College from where he graduated MBBS and MD in Pediatrics. He has done super-specialization in Neonatology from AIIMS, New Delhi.

He is presently on deputation to NITI Aayog as Officer on Special Duty, where in he has been closely associated with various National-level policy works pertaining to Covid Pandemic Preparedness Planning/ Vaccination, Medical Education and Institutions, Human Resource development, Transformation of Trauma & Emergency Care Services, Early Childhood Development, Costing Packages, etc.

In his previous appointments, the officer has been Professor of Pediatrics and a recognized UG and PG teacher at MUHS, WBUHS. He has been Head of Departments of Pediatrics at Command Hospitals Pune and Kolkata.

He is also an avid online teacher for various Neonatology-related courses both in India and abroad. He has numerous publications to his credit both in Indian and International journals.

Talk synopsis

Paradigms of Transforming Health by integration of Science-Technology-Policy and the Way Forward

Bioengineering is a rapidly progressing new field, which necessitates close interaction of clinical specialists, public health experts, biologists and technologists of various domains. To present a holistic picture from a clinical

perspective, an illustrative example of Neonatal Jaundice is discussed, as this medical condition has reaped benefits from advancement in bioengineering- with detailed studies of related fields such as: Physiology, Pathology/ Pathophysiology, Biology, Clinical Sciences, Public Health relevance, Chemistry/ Enzymology, Basic Physics, Applied Physics, Bio-design, Data analytics, Artificial Intelligence, Biostatistics, amongst others.

While the typical historical course taken in the case of arriving solutions for managing Neonatal Jaundice has been in the sequence of *Clinical Sciences – Biology – Technology*; a point is made of other discoveries/ inventions in the field of bioengineering with varied permutations and combinations of these three domains.

For taking the next steps in advancement in the field of bioengineering, India needs to develop enabling ecosystem for medical professionals, engineers, scientists, entrepreneurs and policy makers. This will help in overcoming otherwise tardy course as exemplified in the case of Neonatal Jaundice and which was surmounted in the case of recent COVID pandemic. The logical way forward is to develop close network collaboration of medical and engineering institutions/ professionals by revamping the educational curricula/ developing partnership models, along with integration of explosive technologies.

Dr. Prasad S. Kulkarni, MD, FAP
Executive Director
Serum Institute of India Ltd.,212/2, Hadapsar,
PUNE – 411 028, INDIA
Email: drpsk@seruminstitute.com

Profile:

Dr. Prasad S. Kulkarni, is a graduate (MBBS) and post-graduate (MD) of B.J. Medical College, Pune with specialization in Clinical Pharmacology. He joined Serum Institute of India Ltd. (SIIL), Pune in 2000, and is now its Executive Director. Today, Serum Institute is the largest manufacturer of vaccines in the world.

Dr. Kulkarni has several years experience in clinical research, medical advice and pharmacovigilance. His special focus has been on clinical development of new vaccines and large molecules at SIIPL.

He has more than 70 publications in journals like the *New England Journal of Medicine, Lancet Infectious Diseases, Clinical Infectious Diseases,* etc. He has delivered several lectures in many national and international conferences, workshops and seminars.

Dr Kulkarni has been a faculty to the annual Indian Vaccinology Course (INDVAC) at Christian Medical College, Vellore since 2010. He has been a referee to many international medical journals. He has guided many students in clinical research.

He is also a fellow of the American College of Clinical Pharmacology (FAP). He was recently involved in the clinical development of Covishield and Covovax that played an important role during the Covid-19 pandemic.

Talk synopsis

Enteric fever: Development of a typhoid-paratyphoid A conjugate vaccine

Prasad S Kulkarni

*Serum Institute of India Pvt Ltd., Pune, India; *Correspondence:*

Enteric fever, majorly caused by Salmonella typhi and Salmonella paratyphi A is a serious public health problem with significant morbidity in the developing world. Every year there are an estimated 4.5 million cases in India. Though, typhoid conjugate vaccines are currently available for prevention of typhoid fever, no vaccines against paratyphoid fever are currently available. S. paratyphi A causes almost 90% cases of paratyphoid fever. Therefore, a bivalent conjugate vaccine targeted against typhoid and paratyphoid A has been developed in India. This vaccine comprises of Vi antigen from S. typhi conjugated to tetanus toxoid and S. paratyphi A conjugated to diphtheria toxoid. Single and repeated dose toxicity studies in rats and rabbits showed that the vaccine is safe and immunogenic. Currently, a double-blind, randomized, active-controlled Phase 1 clinical study is ongoing in 60 healthy adults to assess safety and immunogenicity in comparison to Typbar-TCV. The immunogenicity is assessed by estimation of anti-Vi IgG and anti-Vi IgA serum antibodies by ELISA for typhoid antigen, anti-LPS IgG antibodies by ELISA and serum bactericidal assay titres for paratyphoid A antigen. Safety will be evaluated by monitoring solicited events, unsolicited events and serious adverse events. The total safety follow up will be for 181 days. If the study results are satisfactory, this vaccine will be evaluated in further clinical trial phases. This bivalent vaccine can be an effective tool against the problem of enteric fever.

Keywords: Typhoid; Paratyphoid; Vaccines; Enteric Fever

Dr. Chetan Gadgil
Scientist
CSIR - National Chemical Laboratory (NCL), Pune

Profile:
Dr Chetan Gadgil studied Chemical Engineering at UDCT Bombay (now ICT), IIT Bombay and the University of Minnesota. After his PhD he was a postdoctoral researcher at the Mathematics department at the University of Minnesota. He then worked in the US-based R&D division of the British pharmaceutical company GlaxoSmithKline (GSK) before joining NCL Pune as a scientist, and subsequently accepted a joint scientist position at IGIB New Delhi. His research group works on application of mathematical modelling and data analysis to biological systems at scales ranging from intracellular reactions to pharmacology. He has also served in several academic evaluation and administration roles, as Associate Dean (Engineering) in AcSIR, as a member of SERB and DBT committees, and currently as the Head of the Chemical Engineering and Process Development Division at NCL.

Talk synopsis
Mechanism based mathematical analysis of biological processes

Mathematical modelling and data analysis are essential tools for a bioprocessing engineer, and a modern biologist. Models that are formulated based on knowledge of the biological system being studied, as distinct from ‘black-box’ models, are especially useful in studying the typical noisy and limited data arising from experiments. Through examples from research at NCL, I will show the utility of mechanism-informed modelling and analysis in organising data and

formulating testable predictions on the functioning of biological systems. Such models have been applied at NCL to study diverse processes. In some situations, data may be available but appear confusing, and data-based models customised for the experiments must be devised. In some cases, the data may be contradictory, and a model may suggest an explanation for such seemingly unintuitive results. In other situations, when a model is not available, other models developed for a different application may be extended and repurposed to suggest answers to these new questions with existing data. Using our work on skin pigmentation, regulation by microRNA, and tuberculosis drug distribution, I will illustrate the use of mathematical modelling in all three situations.

Dr. Yash Gupte

Product Manager,JioHealthHub, Navi Mumbai, Maharashtra, India

Profile:

Before venturing in digital health, Yash was a Scientist & Manager Synthetic Biology and A2O at Reliance Industries Limited where he played a key role in several international technology transfers. Yash was an integral part of Molecular Diagnostics at Reliance Life Sciences in setting up automated covid testing facility that could process over 25,000 samples per day. Yash was instrumental in developing 2 RT-PCR covid 19 detection kits that were technically approved by ICMR. Yash completed his PhD in Life Sciences from University of Mumbai and MBA from XLRi, Jamshedpur and is currently a Product Manager at Jio Health Hub.

Talk Synopsis

Geographic and demographic diversity of India brings variety of health challenges and opportunities. Most of the health issues are segmented as communicable diseases, non-communicable disease, maternal & child diseases, vector borne diseases, neurological disorders, mental wellness and life style disorders. To reduce the burden on healthcare professionals and ease of patients, personalization of diagnosis, therapy, surveillance and recovery has become a necessity. Medical wearable devices capture certain parameters and provide real-time health tracking, historical data management and better decision-making for patients and medical professionals. Meanwhile, constantly evolving technologies are modernizing diagnosis. Amalgamation of wearable devices and clinically approved diagnostics will lead to accurate preventive diagnosis. Siloed solutions for each health segment limits the purpose of healthcare and therefore digital platforms play a key role in connecting healthcare stakeholders and completing the phygital journey of each stakeholder.

Prof. Srinivasan Ramakrishnan
Assistant Professor,
Indian Institute of Technology, Bombay

Profile:

Srinivasan Ramakrishnan is an electrochemist by training, working at the cutting edge ofadvanced batteries, electrocatalysts for fuel production, and brain-machine interfaces(BMI). He is currently an Assistant Professor of Chemistry at IIT Bombay. Previously, hewas the Electrochemical and Materials Engineering Lead at Neuralink Corporation, anElon Musk-founded company at the forefront of BMI technology. At Neuralink, he ledthe battery engineering and development program along with materials development for*in vivo* neural recording and stimulation. Srinivasan received his PhD from StanfordUniversity in 2017 for his thesis on the design of new electrocatalysts for CO_2 reductionto energy-dense fuels. Following his PhD, he worked as a postdoctoral scholar in theChemical Engineering department at the University of California Berkeley on the surfacepassivation of high-energy Li-ion battery cathode materials for electric vehicleapplications in partnership with LG Chem. Srinivasan has won several awards andfellowships for his work including the Rising Environmental Leaders Fellowship(Stanford University), Center for Molecular Analysis and Design Fellowship (StanfordUniversity), Institute Silver Medal for Best Academic Performance (IIT Madras), andmost recently the Ramanujan Fellowship from SERB (declined). His current researchinterests include the stabilization of electrochemical interfaces in high-energy and highpowerbatteries, implantable electrodes, and catalytically active surfaces.

Talk synopsis

The Promise and Challenges of Neurotechnology

Prof. Srinivasan Ramakrishnan

The electrical interfacing of the central and peripheral nervous system of the human body, broadly termed neurotechnology, is opening up uncharted territories of diagnostics, therapeutics and rehabilitation in patients suffering from brain or spinal cord related injuries. A cutting-edge brain machine interface is a confluence of materials science, electrochemistry, neuroscience, electrical and mechanical engineering among other fields. The talk will broadly cover the promise of state-of-the-art neurotechnological applications, architecture of flexible polymer-based neural probes, and highlight challenges in miniaturization, long term chronic implantation and multi-modal mapping of the electrophysiological activities of neurons.

Dr. Nathan T. Johnson
Investigator at H3 Biomedicine,
Greater Boston

Profile

Nathan Johnson is currently an Investigator at H3 Biomedicine. H3 Biomedicine is a privately held biopharmaceutical company focused on the discovery and early development of novel, targeted anti-cancer compounds for the unmet needs of genetically defined patient populations. H3 has leveraged its integrated expertise in genomics, tumor biology, bioinformatics and innovative synthetic organic chemistry to create an integrated drug development ecosystem to deliver patient-based, genomics-driven, small molecule drugs.

As a former Research Scientist at Harvard Medical School (HMS) and Dana-Farber Cancer Institute (DFCI), he was responsible for merging his biological expertise with computer science and data science in order to achieve breakthroughs in breast cancer and Alzheimer's therapeutic research. He used AI in order to drive new insight into how to recognize relevant patterns that would be difficult to impossible without it. He has been involved in research for almost 15 years across a number of challenges for diseases such as Duchenne Muscular Dystrophy, Polycystic Kidney Disease, Acute Lymphoblastic Leukemia, and on how to prevent parasites from infecting soybeans. Prior to pursuing his graduate studies, he worked as a microbiologist testing food products such as Hershey's, baby formula, and meat for pathogens. He holds a BS in Biology with a minor in Chemistry from Evangel University in Springfield, MO, an MS in Biomedical Sciences from the University of Missouri in Columbia, MO, and a Ph.D. in Bioinformatics and Computational Biology from Worcester Polytechnic Institute (WPI) in Worcester, MA.

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6TH INTERNATIONAL CONFERENCE ON RECENT TRENDS IN BIOENGINEERING (ICRTB-2023)

(January 20 – January 21, 2023)

Detailed Schedule

Day 01: January 20, 2023, Friday

8.30 am to 9.30 am	Spot registrations, arrival of guests, speakers and delegates
9.30 am to 10.30 am	Inaugural program presided by Hon Vishwanath Karad sir, Founder MIT Group of Institutes and President MIT-ADT
9.30 am to 9.35 am	Welcome of audience by the anchors, World Peace prayer and
9.35 am to 9.45 am	Introduction of guests and conference theme by Convenor Dr. Renu Vyas
9.45 am to 9.50 am	Welcome speech by Prof Vinayak Ghaisas Founder Director, MIT
9.50 am to 10.00 am	Brief remarks by the Chief Guest and guest of honour
10.00 am to 10.10 am	Speech by Prof Mangesh Karad, Executive President and Vice chancellor, MIT ADT
10.10 am to 10.20 am	Motivational Talk by Hon. Dr. Vishwanath Karad sir, Founder MIT
10.20 am to 10.25 am	Release of abstract book by dignitaries on the dais
10.25 am to 10.30 am	Vote of Thanks
10.30 am to 10.45 am	Inauguration of poster session and industry stalls by guest followed by Tea break and group photo
11.00 am to 1 pm	Plenary Session I
11.00 am to 11.30 am	Dr. Mohan Wani, Director, NCCS, Pune
11.30 am to 12 .00 pm	Dr. Taslimarif Saiyed, Senior vice president, CEO and Director, C-Camp, Bengaluru, India

12.30 pm to 1:00 pm	Prof. Jeremy Simpson, Dean Academics, University College of Dublin, Ireland
1.00 pm to 2.00 pm	Lunch Break , e-poster session and Industry Expo
2.00 pm to 4 pm	Plenary Session II
2.00 pm to 2.30 pm	Dr. Gagandeep Kang, Professor, Christian Medical College,
2.30 pm to 3.00 pm	Dr. Chetan Gadgil, Scientist, CSIT-NCL, Pune
3.00 pm to 3.30 pm	Dr. Sangeeta Kale, DIAT, DRDO, Pune
3.30 pm to 4.00 pm	Dr. Prasad Kulkarni, Executive Director, Serum Institute of India PVT. Ltd, Pune, India
4.00 pm to 4.30 pm	Prof. Srinivasan Ramakrishnan, IIT, Bombay
4.30 pm to 4.45 pm	Tea break
4.45 pm to 6.00 pm	Oral and Poster presentations by delegates (parallel sessions)
6.00 pm	Day One conclusion

Day 02: January 21, 2023, Saturday

9 am to 11am	Plenary Session III
9.00 am to 9.30 am	Dr. Natalie Artzi, Principal Research Scientist, MIT Institute of Medical Engineering & Science, Cambridge,
9.30 am to 10 am	Dr. Kirsten Sinclair Rosselot, Director, Process Profile,
10 am to 10.30 am	Prof. Justin Dauwels, TU Delft University of Technology,
10.30 to 11 am	Dr. Pawan Dhar, Professor, JNU, New Delhi, India
11.00 am to 11.15 am	Tea Break, e-poster session
11.15 am to 1.00 pm	Plenary Session IV
11.15 am to 11.45 am	Prof. Reza abbasi-Asl, Bioengineering & Therapeutic Sciences University of California, San Francisco USA
11.45 am to 12.15 pm	Dr. Nathan Johnson, Investigator, H3 Biomedicine Associate Research Scientist, Harvard Medical School MA, USA
12.15 pm to 12.45 pm	Dr. Jitendra Sharma, Managing Director & CEO, AndhraPradesh MedTech Zone, India
12.45 pm to 1.15 pm	Dr. Rahul Bhambure, Senior Scientist, CSIR-NCL, Pune, India
1.15 pm to 2.00 pm	Lunch break and poster sessions
2.00 pm to 4.00 pm	Plenary Session V

2.00 pm to 2.30 pm	Brig (Dr.) K. Venkatnarayan, Officer on special duty, NITI Aayog, New Delhi
2.30 pm to 3.00 pm	Dr. Andreas Bender, Digital Life Sciences at innovation Campus Berlin (ICB)/Nuvisan, Berlin, Germany Pvt Ltd
3.00 pm to 3.30 pm	Dr. Yash Gupte, Product Manager, JioHealthHub, Navi Mumbai, Maharashtra, India
3.30 pm to 4.00 pm	Dr. Atul Kurani, Vice Precedent and Head, Medical and IoT Business, Capgemini
4:00 pm to 4.15 pm	Tea break
4.15 pm to 5.15 pm	Oral presentations by delegates (parallel sessions)
5.15 pm to 5.45 pm	Valedictory function, announcement of Prizes, feedback from delegates, concluding remarks by Director, National Anthem
5.45 pm	Conclusion of the event

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Oral Presentations

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Eco-friendly LDPE degradation by Microbes (Bacteria, Fungi) from garbage soil

Pratiksha Guthe and Savita Kate

Department of Biotechnology, Shivchhatrapati College, Aurangabad-431001 M.S, India

Abstract: Plastic and polythene waste accumulating in the environment due to their high molecular weight, hydrophobic nature, high C-C crosslink bonding, make it non-biodegradable and harmful to environment and living organisms. In the present study, we have isolated 19 bacteria and 8 fungi from dumped garbage soil on nutrient agar and PDA at 37◦C, 30◦C after 24h and 3 days incubation respectively. In primary screening, 8 bacterial and 2 fungal isolates were hydrolyzed hydrocarbons (Starch, gelatin) efficiently by zone of hydrolysis (8 to 29 mm of starch, 14 to 38mm of gelatin). Complex hydrocarbons such as Tween 80, Petroleum ether, Naphthalene powder are proficiently utilized by I8, I10 and I13 bacterial isolates and consortium for their growth and it's confirmed their ability to LDPE biodegradation. Bacterial isolates were identified as Bacillus subtilis, Bacillus amyloliquefaciens, and Bacillus licheniformis as per Bergey's Mannual, ABIS software and molecular identification and fungi was identified as Aspergillus sp. Biodegradation of LDPE 81±3.2% weight loss by Bacillus licheniformis, 76.77±1.2% by Bacillus subtilis (I8), consortium 76.88±2.6% and Aspergillus sp. 53.86±6.7% and lowest weight loss 16.18±2.9% was by Bacillus amyloliquefaciens in without glucose minimal media. LDPE utilization for growth by microbes was analyzed by colorimetric method and confirmed with the help of FTIR and GC-MS analysis. Hence in present work, LDPE sheets are eco-friendly biodegraded by isolates helps in reducing environment pollution.

Keywords: polythene, biodegradation, hydrocarbon, FTIR.

Impact of clomazone on acetylcholinesterase and lipid peroxidation upon exposure to freshwater fish

Kalpana Singh* and Vandana Garg

Department of Zoology, D. N. (P.G.) College, Meerut
*Corresponding author: ksingh0696@gmail.com

Abstract- In this study, the freshwater fish Channa punctatus was used to study the harmful effects of clomazone on AChE and LPO at three different doses and for four different exposure times. To determine the sublethal concentrations of clomazone, the LC50 of the herbicide was calculated. Based on the calculated LC50 value, three different concentrations were determined: high dose- 0.5 ppm, mild dose- 0.25 ppm, and low dose- 0.08 ppm. The fish were treated with these concentrations and the exposure period was 7, 14, 21, and 28 days respectively. The acetylcholinesterase activity and concentration of MDA were significantly decreased ($p<0.05$) and increased ($p<0.05$), respectively, upon higher concentration and also with the increase in exposure periods. The highest reduction of AChE was recorded in the liver, followed by the kidney and gill in all three concentrations. On the other hand, the MDA concentration was recorded highest in the kidney, followed by the liver and gills. Though, in the liver, the concentration of MDA is almost the same when exposed to concentrations of 0.5 and 0.25 ppm clomazone. Thus, our findings imply that AChE activity and lipid peroxidation may be potential indicators of environmental pollutants in aquatic systems.

Keywords: AChE, Clomazone, Channa punctatus, MDA, Tissues.

A Carbon Quantum Dots (CQDs) -Glucose Oxidase (GOX) based biosensor for the specific detection of copper heavy metal ions in various water matrices

Tanmay Vyas and Abhijeet Joshi*

Department of Biosciences and Biomedical Engineering, Indian Institute of Technology Indore, Khandwa Road, Indore- 453552, Madhya Pradesh, India

Abstract: Environmental pollution is one of the worrying issues now a days all over the globe, due to this several hazardous effects causes to environment and all the species. Many pollutants cause water pollution, one of the chief pollutants of water pollution are Heavy metal. Heavy metal toxicity and pollution in water resources has great concern for entire globe. Heavy metal above their permissible limit causes various health issue to us. The detection of heavy metal is necessary for the treatment and removal of heavy metal from the water resources. Copper is one of the most toxic heavy metals causes several health hazardous effect like carcinogenic, nephrotoxic, neurotoxic effects to population. This research demonstrates the synthesis and characterization of carbon quantum dots (CQDs) thin film immobilized with glucose oxidase (GOX) for the fluorescence based specific detection of copper heavy metal with good linearity and accuracy along with minimal limit of detection (LOD) and short response time. This research approaches towards the point of care monitoring with real time potable sensing of copper heavy metal ions for environmental monitoring.

Key words: Carbon Quantum Dots (CQDs), fluorescence, fiber optic spectrometer, heavy metal pollution, water resources.

Discovery of black cumin mediated drug molecules as a potential natural inhibitor for Covid-19 by molecular docking and dynamic simulation studies

Md. Ahad Ali[1,2], Md. Selim Reza[1], Harun-or-Rashid[1], Humaira Sheikh[3], Md. Mahbubor Rahman[2], Md. Nurul Haque Mollah[1]*

[1]Bioinformatics Lab (Dry), Department of Statistics, University of Rajshahi, Rajshahi 6205, Bangladesh
[2]Department of Chemistry, Faculty of Science, University of Rajshahi, Rajshahi 6205, Bangladesh
[3]Department of Chemistry, Bangabandhu Sheikh Mujibur Rahman Science and Technology University, Gopalganj.
*Corresponding Author: mollah.stat.bio@ru.ac.bd

Abstract: The SARS-CoV-2 was identified in 2019 as the COVID-19 causing virus, which is now a global pandemic. Black Cumina is a seasonal plant that belongs to the family of Ranunculaceae native to Southwest Asia. The purpose of this study was to identify black cumin mediated potential candidate drug molecules for the treatment against Covid-19. Here, we investigated approximately eleven target proteins (ACE2, RdRp, Spike,3CLpro, MAPK8, TMPRSS2, PLpro, IL6, N, TNF, NFKBIA) from our study and 59 meta drugs compounds of black seed (Nigella Sativa) and finally we found alpha-Sitosterol, Rutin, alpha-Spinasterol & Isoquercitrin as the top-ranked four candidate meta drugs with the highest binding affinity from the docking study by PyRX software. The drug-likeness properties of phytocompounds were studied using pkCSM and SwissADME online web tools. We performed 100ns molecular dynamic simulations by Yasara (version 22.9.24) to assess the constancy of docked complexes and found their stable performance. This MD-based MM-PBSA simulation showed the drug's stability with the suggested top-ranked target protein with four ranked drugs. Finally, we calculated the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), and energy gap values using density functional theory (DFT) through Gaussian 09. From the docking and ADMET study, four top-ranked compounds, Alpha1-Sitosterol, Rutin, Alpha-Spinasterol, Isoquercitrin, were important interacting ligand with ACE2, RdRp, 3CLpro, and, S(Spike) for COVID-19 interaction is significantly higher than other proteins. The findings of this study showed that Alpha-Sitosterol, Rutin, Alpha- Spinasterol, and

Isoquercitrin might be considered as the potential lead compounds for COVID-19.

Keywords: Black cumin, SARS-CoV-2 infection causing genes, Molecular Docking and dynamic MD Simulations

Synthesis of Folic Acid Tagged Superparamagnetic Iron Oxide Nanoparticles for pH Responsive Drug Delivery

Md Ahad Ali, Md Shahidul Islam, Hasan Ahmad and, Md Mahbubor Rahman*

Polymer Colloids and Nanomaterials Laboratory, Department of Chemistry,
Faculty of Science,
University of Rajshahi, Rajshahi-6205 Bangladesh
*Corresponding author: s1710423104@ru.ac.bd; ahad.chembd@gamail.com

Abstract: In the area of drug delivery, controlling the release of therapeutic substances at localized targets has become one of the most prominent areas of medical research, especially in the treatment of cancer. The biocompatibility and (super) paramagnetic properties of iron oxide nanoparticles (IONPs) make them one of the most promising drug carriers. In this study, the synthesis of folic acid (FA) conjugated hyperbranched polyglycerol (PG) coated iron oxide nanoparticles (SPION- PG) is envisioned. For biological SPION-PG is converted into SPION-NH_2 via (SPION- PG→SPION-TsCl → SPION-N3 → SPION-NH_2). It is hypothesized that (SPION-NH_2) coating on IONPs and FA conjugation with PG will induce the NP's high water dispersibility and affinity to cancer cells via folate receptor respectively. The pH-responsive delivery of doxorubicin (DOX) drug in vitro will be studied using nanoparticles following their synthesis. A hydrazine bond will be incorporated into polymers by functionalizing the -OH groups from the polymers into the -NH 2 groups. Consequently, the chemically linked or covalently linked DOX will hydrolyze under acidic conditions (<5.5), releasing the drugs in a pH-sensitive manner.

Keywords: Iron oxide nanoparticles; hyperbranched polymer: folic acid; drug delivery; anticancer drugs; pH-Responsive.

Comparison of Various Synthesis Approach of Zinc Oxide Nanoparticles for Enhanced Antimicrobial activity

Shraddha Jaiswal and Vidya Tale*

Department of Microbial Biotechnology, Rajiv Gandhi Institute of IT and Biotechnology Pune India

Abstract. The aim of our investigation is to compare different synthesis approaches of Zinc oxide (ZnO) nanoparticles and their antimicrobial efficacy against pathogenic bacteria. The synthesis process was carried out by chemical method Sol gel, Co-precipitation with oxalate, Polyol and Green synthesis using Triphala extract. All synthesized ZnO nanoparticles were characterized by UV visible spectroscopy (UV), Dynamic light scattering-Zeta potential, X-ray diffraction (XRD), and fourier transform infrared spectroscopy (FTIR). Different levels of antibacterial and antibiofilm action were demonstrated by all nanoparticles against different strains of Gram-positive Staphylococcus aureus and Gram-negative Pseudomonas aeruginosa. The antibacterial activity was found to be inversely related to the particle size and calcination temperature of the synthesized ZnO nanoparticles. Among all methods, ZnO nanoparticles with least size was achieved by sol gel method using precursor as zinc acetate dihydrate with lower calcination temperature, demonstrated impressive antibacterial action, suggesting possible alternative for biomedical application

Keywords: Zinc Oxide Nanoparticles, Sol gel, Co-precipitation, Triphala

In silco method to design immunotherapeutic for cancer treatment

Manoj Sabnani, Renu Vyas, Neeraj Maheshwari, Sanket Bapat

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Abstract: New treatment regimens for cancer are being explored due to off-target effects of chemotherapy and radiation therapy. Immune cells express multiple types of membrane receptors which engage with different extracellular ligands on the tumor cells and lead into activation or deactivation of immune response. This interaction between receptor and ligand not only accumulates immune cells in the tumor microenvironment but also triggers different cell signaling pathways. Monoclonal antibodies against inhibitory pathway is PD1-PDL1 axis on tumor cells, or CTLA-4 are one of the few emerging therapies developed in last two decades. Immunotherapy drugs called immune checkpoint inhibitors work by blocking checkpoint proteins from binding with their partner proteins. This prevents the "off" signal from being sent, allowing the T cells to kill cancer cells. Some tumors turn down the T cell response by producing lots of PD-L1. Anti PD1 antibody can break this nexus between PD1 (on the T cells) and PD-L1 overexpressed on the tumor cells, resulting into targeting of cancer cells by cytotoxic T cells.

We will discuss a new model to simulate the binding process between multi-specific ligands and membrane receptors on cell surfaces. In this study, we analyzed 32 FDA approved sequences of anti PD1 antibodies from the TABS database. We used structural modelling in conjugation with molecular docking and MD simulation to discover and redesign single domain antibodies (VHH) against the same target with improved affinity and specificity. Complementarity determining regions (CDRs) targeting PD1 were grafted onto structurally matched antibody scaffolds. We designed and tested in silico three single-domain antibodies (VHHs) targeting Program death 1 (PD1/PDL1) antigen. Insilco characterization showed that all designs are highly stable and bind PD1/PDL1 with sub nano molar binding affinities (KDs). This method will help to discover stable VHHs with sub nanomolar KDs without in vitro affinity maturation. Future applications of our method will pave the way for new strategies to generate next-generation biologics.

Quercetin- Next bioactive super molecule scope with adjuvant

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Quercetin is a flavanoid found common in some healthy fruits and vegetables/ spices such as Red Onion, Coriander, Pomegrenate, Tea, Coffee, Ashwagandha (Indian Ginseng) etc. It is found to be highly anti-inflammatory and sold today as over the counter food or health supplement in the western world to lessen the intensity of many lifestyle ailments such as cardiovascular, hypertension and diabetes. Curcumin is another bioactive super-molecule emerging in the past decade, obtained from the famous Indian spice Turmeric. It is promoted globally today as the smoothie "Turmeric latte" as anticancer, anti-inflammatory health supplement, an over the counter (OTC) product. However, its bioavailability is low so large amounts need to be consumer for medicinal effect. But its "hot" vide traditional wisdom and caused side effects- such as pimples, boils, blood letting in stool/ piles. Its an organic molecule not water soluble, and is batter absorbed in fat medium such as milk or butter/ Ghee (clarified butter). Turmeric water decoction is also promoted as health drink abroad but with uncertain results. Quercetin anti-inflammatory potential is higher (binding energy -9.93 Kcal/ mol) than Curcumin (binding energy -8.7 Kcal/ mol) vide docking study we got done at Pune at Rasa Life Sciences co. Similar results are found in Russia and Saudi Arabia that rank Quercetin among the highest among the bioactives. Quercetin is not yet found to have conclusive medicinal evidence in large scale or multi-country trials and the results so far are limited to pre-clinical trials confined to about hundred patients or less. It is found ineffective even in some such limited tests but having better, curative effect even in COVID-19 when jointly administered with adjuvant such has vitamin C. It is also found senolytic and being tested for anti-aging effect along with Dasatinib. Thus, adjuvant molecules need to be tested along with quercetin for better efficacy in future studies. Nanotechnology may be another strategy to improve bioavailability such as Ayurvedic decoctions named as "Asava" or "Arishta' or "Bhasma"or "Bhasma". Aspirin, Menthol, Morhine have been some of the multi-billion dollar super-molecules derived from plants (Birch tree bark, Mint herb, Poppy weed etc.)

thus far, used to treat fever, cough, pain etc. respectively. These are found useful singularly but new molecules nay need new drug delivery strategy.

Synthesis and 3-D Bioprinting Efficacy of highly-reproducible Bioink for Skin- Tissue Regeneration

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Abstract: 3-D Bioprinting is employed as a novel approach in biofabrication to promote skin regeneration following chronic-wounds and injury. A novel bioink composed of carbohydrazide crosslinked {polyethylene oxide-co- Chitosan-co-poly (methylmethacrylic-acid)} (PEO-CS-PMMA) laden with Nicotinamide and human dermal fibroblast was successfully synthesized via Free radical-copolymerization at 73 ^{o}C. The developed bioink was characterized in term of swelling, structural-confirmation by solid state 13C-Nuclear Magnetic Resonance (NMR), morphology, thermal, 3-D Bioprinting via extrusion, rheological and interaction with DNA respectively. The predominant rate of gelation was attributed to the electrostatic interactions between cationic CS and anionic PMMA pendant groups. The morphology of developed bioink presented a porous architecture satisfying the cell and growth-factor viability across the barrier. The thermal analysis revealed two-step degradation with 85 % weight loss in term of decomposition and molecular changes in the bioink moieties By applying low pressure in the range of 25- 50 kPa, the optimum reproducibility and printability were determined at 37 ^{o}C in the viscosity range of 500-550 Pa. s. A higher survival rate of 92% was observed for (PEO-CS-PMMA) in comparison to 67 % for pure chitosan built bioink. A binding constant of K≈ 1.8 X 10^{6} M^{-1} recognized a thermodynamically stable interaction of (PEO-CS-PMMA) with the Salmon-DNA. Further, the addition of PEO (5.0 %) was addressed with better self-healing and printability to produce skin-tissue constructs to replace the infected skin in human.

Enhanced removal of toxic heavy metals from wastewater using silica-based magnetic nanomaterial

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Abstract: In recent years, the utilisation of waste disposal and byproducts from many industries has drawn more attention in the fields of ecology, science, business, technology, and social welfare. Heavy metal wastewater is immediately dumped into the environment due to the industry's rapid development. They accumulate inside living things, are harmful to health, and are not biodegradable. Several nanoparticles have been identified by numerous researchers for the removal of heavy metals due to their functionality and improved adsorption capacity and effectiveness. Nanomaterials with a silica coating can be utilised to remove heavy metals. Rice Husk, a common waste product of Rice milling is an abundant source of Silica. The primary factors in favour of using rice husk are its granular structure, chemical stability and accessibility locally at a very low price. In rice-growing nations including India, China, Brazil, the USA and Southeast Asia, rice husk is widely accessible. Rice Husk Ash is produced by burning the rice husk. To create pure silica xerogels from RHA, alkaline extraction was carried out accompanied by acid precipitation. Silica-coated Fe3O4 magnetic nanoparticles were synthesized via microwave technique and were used for the elimination of Cr (IV) ions from the samples of water. The magnetic nanoparticles that are synthesized were differentiated using Scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier- transform infrared spectroscopy (FT-IR), Dynamic Light Scattering (DLS), and Zeta Potential. The effect of variables like pH, temperature, time of contact, and the target metal ion concentration was constantly monitored using Atomic Absorption Spectroscopy (AAS) to obtain optimum conditions.

Keywords: Rice husk, rice husk ash, nanoparticles, silica xerogels, heavy metals, magnetite, microwave, nano- adsorbent, water treatment.

Evaluation of the immobilization factors affecting tannase activity by statistical experimental design

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Abstract: Tannin acyl hydrolase (3.1.1.20) or tannase, is a hydrolysable, tannin degrading enzyme; as tannin is hazardous to the environment, removal of tannin containing materials from environment is a burning issue and required ecofriendly technologies for degradation and complete removal of them using suitable enzyme. Tannase., is an inducible enzyme and has a wide range of applications in foods, animal feeds, cosmetics, pharmaceuticals, chemical and leather industries. It is still considered as a novel and one of the costly enzymes.
Recognizing the importance of enzyme. The present study aims to explore the statistical techniques and improve the immobilization process of tannase produced by Streptomyces variabilis (SKA1). Use of immobilized enzymes overcomes many practical difficulties. Statistics and experimental designs are important tools for the field of life science and should be used while planning, conducting research experiments as well as during the analysis and interpretation of results.
In the present investigation, use of sodium alginate as a carrier for immobilization exhibited high enzyme activity, therefore the Plackett-Burman experimental design; a fractional factorial design was applied to know the importance of various immobilization factors on the production of tannase. The analysis showed that only calcium chloride had a significant influence (at 95% significant level) on enzyme activity.

Keywords: Tannin, hazardous, tannase, immobilization, statistical design, importance

Nano-biotechnological approach for sustainable disease management in sugarbeet cultivation under changing climate

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Abstract: Sclerotium rolfsii is most destructive fungi in sugarbeet (Beta vulgaris L.), causes sclerotium root rot and responsible for about 50% damage of roots. Affected roots are unfit for sugar extraction causing major economic loss. Applications of chemical fungicide to manage the disease, cause serious environmental hazards of flora, fauna and human. Now a days, climate change is major problem and has a severe impact on the incidence of erratic, extreme weather events leading to substantial effects on the ecosystems. Efforts are therefore required for enhancing crop resilience and adaptation to climate change for sustainable agriculture production. The changing climate is unpredicted and increased diseases and pest infestations; thereby impose severe risks and potential crop failures. To tackle this problem, we synthesized chitosan and β- glucan nanoparticles (yeast and S. rolfsii β- glucan) in order to enhance plant immune stimulation against the pathogenic fungi S. rolfsii. Synthesis of nanoparticles was confirmed through FTIR, FE-SEM, TEM- EDS, XRD zeta size and zeta potential techniques. In-vitro antifungal study of these nanoparticle indicates that chitosan and both β- glucan nanoparticles able to inhibit 100% of S. rolfsii growth at 600 ppm and 160 ppm respectively. Antifungal activity of nanoparticles also tested in Czapek- Dox liquid media, in that change in pH and dry weight recorded. Microscopic study shows that nanoparticle causes serious cytoplasmic leakage, cell wall disruption, necrosis and reduction in cytoplasm amount due to its leakage and coagulation in S. rolfsii. This preliminary research will help in developing a nano formulation strategy for sustainable disease management in sugarbeet.

Keywords: β- glucan nanoparticles, chitosan nanoparticles, climate change, Sclerotium rolfsii, sugarbeet.

Prediction of antimicrobial activity in short-chain peptides based on their physico-chemical properties using random forest

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Abstract: Antimicrobial peptides (AMPs) have exhibited an effective and widespread impact in healthcare for evolving into a novel strategy against bacterial infections which have become immune to most of the conventional antibiotics. In-silico approach of evaluating antimicrobial activity for multiple combinations of peptide sequences proves to be optimizational in terms of time and effort when compared to wet lab analysis. In the current study, we have developed a predictive machine learning model which incorporates the physico-chemical and spatial properties of peptide sequences. We propose that the amino acid composition, α-helix and β-sheet propensities, charge-to- hydrophobicity ratio, isoelectric point and their dipeptide composition are significant features that might be useful parameters for identifying novel AMPs. This model utilizes the Random Forest algorithm of predicting which is capable of providing the best accuracy and precision when compared to other techniques. Additionally, we have developed a means of predicting all possible peptide sequences having a maximum length of 10 amino acids with antimicrobial properties. Thus, we constructed an AMP library containing new sequences which can be implemented in-vivo to synthesize novel AMPs that are successful against resistant microbial infections and would overcome the drawbacks of conventional treatment.

Keywords: Antimicrobial peptides, α-helix propensity, β-sheet propensity, charge-to-hydrophobicity ratio, dipeptide composition, random forest model, AMP library, predictive model.

Study to assess the correlation between extracellular enzymes and pathogenicity of *Xanthomonas citri pv. viticola* in grapes

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Abstract: The gram-negative plant-pathogenic bacterium *Xanthomonas citri pv. viticola* is the causative agent of bacterial leaf spot disease which causes economic losses in grapevines. A pathogenic lifecycle faces various challenges exerted by the external environment (both within and outside the host). To successfully colonize the host and establish infection, pathogens had evolved sophisticated systems to combat the host defense mechanisms and also to withstand adverse environmental conditions. In the process of pathogenesis pathogen produces an array of extracellular enzymes. An attempt was made to correlate the extent of extracellular enzymes produced by the pathogen and their degree of virulence. Ten different *Xanthomonas citri* pv. *viticola* strains collected from different locations were screened and quantified for production of extracellular enzymes viz. protease, cellulase, amylase and lipase. Pathogenicity of these 10 *Xanthomonas* strains was assessed *in vivo* under glasshouse conditions by syringe infiltration and pin prick methods. It was observed that all strains had produced the enzymes at varied concentrations leading to variation in symptom expressions. While correlating both the results it was noted that those *Xanthomonas* strains which had produced higher quantity enzymes had manifested more pathogenesis then the other strains. It remains premature to draw any conclusion about the importance of extracellular enzymes in plant pathogenesis, but further studies in this domain will aid in understanding the pathogenicity of pathogen and its variability.

Keyword: *Xanthomonas citri pv. viticola*, extracellular enzymes, pathogenesis, virulence

Antimicrobial activity and phytochemical analysis of *Cassia tora* leaf extract

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Abstract: The secondary metabolites produced by the plants are abundant and used in the treatment of a variety of illnesses. Contaminated water and food are significant factors in the spread of the disease, particularly in developing countries. Unavailability of water, polluted water and inadequate sanitation are responsible for the cause of maximum diseases and sickness. *Cassia tora* Linn. (Caesalpinaceae) is a semi-wild annual herb grown widely in different places of southeast Asia including India, Northern Australia and America. This plant species is well known for having potential in traditional medicine practices. The study aimed at exploring the possibility of using the extract of *C. tora* leaves to inhibit the growth of surface water *E. coli*. Most probable number (MPN) analysis of contaminated water with and without extract was performed. The antimicrobial activity was confirmed by disc diffusion method. Maximum inhibition of water borne *E. coli* was observed at 1000 ppm concentration of plant extract. The phytochemical analysis of the extract revealed the presence of flavonoids, tannins phenols and terpenoids.

Key words: *Cassia tora*, surface water *E. coli*, antimicrobial activity, phytochemical analysis

In-silico prediction and multi-targeted molecular docking analysis of approved drugs, investigational drugs, and natural bioactive compounds for MRSA

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Abstract: *Methicillin-Resistant Staphylococcus aureus* (MRSA) is the most prevalent bacterial that causes secondary infection in Indian hospitals due to resistance to beta-lactam antibiotics. For this study, we conceptualized an exploratory project to study the molecular mechanics of MRSA and how it causes antibiotic resistance. Penicillin Binding Proteins (PBPs) are the group of proteins that are targeted by beta-lactam antibiotics, specifically Penicillin. To investigate this in-depth, we developed a computational workflow for molecular docking of antimicrobial drugs to Penicillin Binding Protein-2a (PBP2a) and Penicillin Binding Protein- 4 (PBP4), transpeptidases that catalyze cell wall biosynthesis in the presence of beta-lactam antibiotics. PBP2a plays a significant role in drug resistance to beta-lactams. Several papers have discussed its mechanism, and many drugs to combat it are currently being developed. PBP4, like PBP2a, can also provide high-level and broad-spectrum resistance to the entire class for β-lactam medicines. PBP4's role in β-lactam resistance in S. aureus has been overlooked, and as a result, its mode of action is largely unknown. We investigated the physiochemical, structural, and functional properties of proteins. Then we used AutoDock Vina to perform a virtual screening of 100+ selected compounds against these two proteins, including FDA- approved drugs, FDA-unapproved drugs, investigational-only drugs, and natural bioactive compounds. In silico methods were used to approximate ADME parameters, toxicity risk, and biological activity of those compounds. Through our pipeline, we discovered bioactive substances that could possibly be repurposed for the treatment of MRSA infections.

Keywords: *Methicillin-Resistant Staphylococcus aureus* (MRSA), Penicillin Binding Proteins (PBPs),Molecular Docking, Molecular Dynamics

Effect of bile salt on self-assembled triblock copolymers

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Abstract. Due to its distinct structure and functionality, triblock copolymer micellesare regarded as one of the most promising nano drug delivery methods. Polymeric micelles self-assemble to produce nanoscopic core/shell structures when they dissolvein water. The inner core hydrophobic anhydrous region of the micelle facilitates the solubilization of drug molecules that are water insoluble. To increase the duration of medicine retention, however, it is imperative to address the integrity of the micellarcore structure. Because of their prospective uses in the pharmaceutical industry, bile salt have recently attracted a lot of attention. Bilesalt incorporated triblock polymers are a brand-new class of substances with special qualities that make them perfect for particular medical applications. In this study the efficiency of bile salt in improving the drug encapsulating capability of triblock copolymer micelles will be explored.

Keywords: Polymeric micelle, drug delivery system, bile salt

Biodegradation of lambda cyhalothrin using microorganisms isolated from grape berry surface

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Abstract: Insecticides of the pyrethroid class are extensively employed in agriculture. One of the most regularly utilised pyrethroids is lambda cyhalothrin. Although lambda cyhalothrin is frequently used to combat defoliating insects, particularly beetles, it also has a considerable impact on naturally occurring non-target species. Despite the low toxicity profile of the pesticide in mammals, higher doses are dangerous and can have detrimental effects on their health due to their accumulation. The grape berry surface exhibits a significant and diverse microbial community. Two bacteria, LC1 and LC2, isolated from Thompson Seedless grape berry surface, showed lambda cyhalothrin biodegradation capability in *in vitro* studies. These bacteria not only demonstrated efficient biodegradation in a lab setting, but they were also effective in field experiments. In the field investigation, isolate LC1 degraded lambda cyhalothrin on average by 66.13%, and isolate LC2 degraded it on average by 80.79%. Both the isolate belonged to genus *Bacillus*. Another significant finding from the study was that the biodegradation process was influenced by the initial inoculum concentration of the bacteria, thereby, necessitating the maintenance of the same inoculum by recurrent spraying. These bacteria have the capacity to biodegrade pesticide, which will aid in the development of bioremediation techniques for lambda cyhalothrin decontamination.

Key words: Grape berry, epiphytic microbe, lambda cyhalothrin, biodegradation

Molecular Modeling studies of BBB drugs on astrocytic receptors in Alzheimer's disease

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Abstract: This research project was undertaken to explore the effects of blood brain barrier positive drugs on astrocytic receptors involved in Alzheimer's disease, by evaluating the binding affinity and trajectory of the researched targets against the drugs approved by the FDA for the disease, as well as blood brain barrier positive drugs in order to illuminate the potential of these drugs to treat Alzheimer's. 17 astrocytic targets were retrieved from RCSB Protein Data Bank and analyzed based on extensive literature surveys. 25 drugs were chosen due to their blood brain barrier penetrating capability while also displaying central nervous system activity, along with 4 drugs approved by the FDA for disease treatment. Molecular docking was performed against the chose targets, and the interactions in the complexes were subsequently analyzed using AutoDock Vina, PyMOL and Discovery Studio software and database. The FDA drug Donepezil was found to have a good docking score of -8.6, -8.6 and -8.8 kcal/mol against four of the chosen receptors, and blood brain barrier positive drugs Paroxetine and Paliperidone showed scores of -8.5, -8.9 and -9 kcal/mol. Paroxetine and Paliperidone are potential candidates for repurposing, in order to treat Alzheimer's disease, targeting its affected astrocytes. Using wet laboratory techniques, the obtained results can be further verified and analyzed.

Keywords: Alzheimer's disease, astrocytes, blood brain barrier, paroxetine,paliperidone, molecular docking, molecular dynamics.

Design of a microfluidic system for opticalanalysis of environmental pollutants

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Abstract: The increasing demand for environmental monitoring necessitates in-situ real-time observations. Miniaturized in situ chemical analysers, which use microfluidic technology, have recently emerged as a potential solution to gather this important data. The goal of the study is to create an on- chip chemical reaction module based on microfluidic technology that can mix reagents of varying concentrations with samples to get colorimetric results. An optical sensor was designed to conduct a colorimetric analysis of the assay that had been performed in the microfluidic channels. Using the COMSOL Multiphysics software, the fluid flow patterns, concentration distribution, and velocity field were studied. Based on the findings, the ideal flow channel dimensions are determined, and polydimethylsiloxane (PDMS) is then used to fabricate the channel. A microfluidic device in PDMS was made utilising soft lithography and replica moulding, which can handle aqueous liquids more swiftly and economically than conventional methods. Microchannels for fluid flow and a reservoir with optical fibres embedded for colorimetric sensing comprise the PDMS reactor chip. In this article, we discuss the design considerations for a generic optical sensor that uses microfluidic technology to monitor environmental pollutants.

Computational drug repurposing approach to obtainpotential anti-HEV molecules

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Abstract: Hepatitis E virus (HEV), responsible for acute viral hepatitis, is endemic in Central Asia, Africa and Central America with severity especially high in pregnant women. Side effects of off-label therapies and lack of effective antivirals warrant exploring the existing drugs for anti-HEV activity through drug repurposing. Transcriptome analysis of infected cells to that of control cells allows identifying changes in the gene expression pattern after acquiring disease to get potential drug candidates which would reverse the effect. The study compared these patterns and identified a few potential anti-HEV molecules using a computational drug repurposing approach. Gene mapping of available wet-lab RNA seq data resulted in successful mapping of about 49 to 89 % of genes on the reference genome. 203 up-regulated and 311 downregulatedgenes were obtained. Total 85 drugs (which reverse the altered DEG pattern) were obtained from cMAP using top 150 up and downregulated genes. 15 drugs were finalised by eliminating drugs having low scores, and those without any known animal and cell line toxicity values. Two DEGs, LGALS9 and NRC2 were obtained with associated potential drug candidates and GO (pathway) terms. LGALS9 coding for galectin 1 and galectin 9 protein products affect biological pathways crucial for viral entry in host cell (GO:0046598) and also responsible for regulation of CD4-positive, CD25-positive, alpha-beta regulatory T cell differentiation involved in immune response (GO:0032832). These dictated the identification of the following molecules of high anti-HEV potential: Mercaptoethanol; Thiodigalactoside; 1,4-Dithiothreitol; Artenimol; (R)-1-Para-Nitro-Phenyl-2-Azido-ethanol.

Keywords: Hepatitis E virus, Transcriptome, RNA seq, cMAP, DEG.

A Comparative Chemoinformatics Analysis of compounds extracted from *Nyctanthes arbor-tristis*

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Abstract: Natural products are a rich source of diverse chemical compounds with interesting therapeutic properties. There is a need for in- depth investigation of this reservoir with *in-silico* tools to assert in the molecular diversity with respect to clinical significance. Although studies have been reported on plants such as *Nyctanthes arbor-tristis (NAT)* and its medicinal importance. A comprehensive study on comparative analysis of all phyto-constituents has not been carried out. In the present work we have carried out a comparative study of compounds obtained from the ethanolic extracts of various parts such as calyx, corolla, leaf and bark of NAT plant. The extracted compounds were characterized by LCMS and GCMS studies with interesting results. The most significant observation was that the compounds from calyx and corolla were closer in chemical space to the anti-arthritic compounds. This was further corroborated by the network analysis, docking and dynamic simulation studies with validated anti-arthritic targets. To further expand and explore chemical space, the common scaffolds were seeded to enumerate a virtual library .The virtual molecules were prioritized based on the drug like and lead like scores and docked against anti-arthritic targets to reveal identical interactions in the pocket region. The comprehensive study will be of immense value to medicinal chemists for rational synthesis of molecules as well as bioinformatics professional for getting useful insight in identifying rich diverse molecules from plant sources.

Keywords: *Nyctanthes arbor-tristis*, Natural Products, Chemoinformatics, Molecular Docking, Molecular Dynamics.

Development of a Disease Trigger Prediction Model for Early Diagnosis of Epilepsy

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Abstract: Epilepsy is the third prevalent mental disorders that has a negative effect on patient's lifestyle and poses a severe health risk. In order to treat a disease, it is now crucial for researchers to identify the precise mechanism that generates a specific symptom at an early stage. Due to the fact that earlier detection of any sickness enables one to control the symptoms and prevent the condition, we propose a disease trigger prediction model for patients with epilepsy to anticipate the episodes of the affected person, giving us an accurate idea of when they might experience the symptoms. The study intends to identify such at-risk patients using clinical and demographic data gathered from electronic medical records, thus identifying such patients is not an easy process and necessitates lengthy courses of trial and error strategies. This approach will specifically employ a combination of predictive analytics machine- learning techniques, along with a cutting-edge method for data balancing, to identify patients with epilepsy using their comorbidities, demographic data, and the initial epilepsy-related diagnosis made by their doctor. This can be implemented using Supervised Machine Learning algorithms such as K-fold cross validation algorithm, K-Nearest Neighbor (KNN) algorithm as well as a Deep learning algorithm such as Convolutional Neural Networks (CNN). A clinical decision support system for medical practitioners will be developed using the positive results from the model, highlighting the potential applications of machine-learning techniques in facilitating healthcare decisions.

Keywords: Epilepsy, disease trigger model, machine learning, predictive model, demographic analysis.

Design and Development of Bioinformatics Approach to Optimize Burrows-Wheeler Aligner in NGS Workflow on Big Data Analytics Framework.

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Abstract: The Next Generation DNA Sequencing (NGS) data analysis pipeline involves many steps among which sequence alignment is the most essential and is computationally expensive. To optimize aligner's efficiency and deliver findings in a timely way, various solutions are provided using Hadoop big data frameworks. However, they require technical expertise and coding proficiency or else introduce computing latencies and fail to support conventional bioinformatics tools execution approach. To overcome this, current work is targeted to accelerate alignment steps adopting big data technologies while executing it using traditional bioinformatics methods. We have developed BWADoop, a high throughput approach for improving the performance of the Burrows-Wheeler Aligner BWA algorithm based on Hadoop Map-Reduce implementations and Parallel Distributed Shell processing utilities. The model was deployed on the standalone Hadoop cluster of commodity computers making it cost-effective. The implementation is fully automated by wrapping BWA logic in a single command. The efficiency was evaluated on whole exome samples of ovarian cancer yielding 83 % reduction in run time of alignment step and speedup of 5.8x using 6 data nodes. The model's accuracy was optimized using the fastdoop library achieving a sensitivity value of 0.86 using confusion matrix scores. BWADoop is a highly scalable algorithm delivering improved performance to help researchers expedite their NGS data analysis research and achieve faster results.

Index Terms- Burrows-Wheeler Aligner, BWA, Hadoop, Sequence alignment, NGS, Big data, PDSH, Confusion

An optimized deep learning network for automatic classification of COVID-19, pneumonia, and tuberculosis from X-rays

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Abstract: Chest imaging is the primary step in detecting anyone with pulmonary and infectious symptoms during the COVID-19 pandemic. The main side effect of the illness is pneumonia, and the new Corona infection has morphology toward slower breathing. The demand for quick testing, diagnosis, and treatment is rising as the worldwide coronavirus disease pandemic of 2019 (COVID-19) continues to have a substantial impact on the health of the global population. The COVID-19 virus can cause severe pneumonia, so early detection is crucial for the right course of treatment and to ease the burden on the healthcare system. In addition to COVID-19, the medical system is also challenged by other pneumonia and tuberculosis (TB) aetiologies. A constant estimate of the most significant cause of childhood death is pneumonia, which can be both viral and bacterial. It kills roughly 2 million infants annually (according to the World Health Organization). The main imaging modalities for identifying respiratory illnesses are computed tomography (CT) and chest X-rays (CXR). Despite being the gold standard, CT scans are more expensive, time-consuming, and come with a minimal but significant radiation dosage. CXR have therefore become more common as a first line examination. To address these problems, the current study has intended to develop deep networks with optimization technique in order to provide the best severity analysis results using Assessment tool. Finding the detection of diseases for COVID, pneumonia and TB is the main goal of the current study project. In order to do such, the current study has developed a revolutionary black widow optimization-based radial basis neural (BWORBN) framework. Pre-processing, feature extraction, affected portion segmentation, disease detection, and classification are the processes that have been incorporated into the currently proposed system. In order to confirm the superiority of the suggested work, the performance of the constructed model has also been evaluated by measuring the detection parameters and compared with other recent related work.

Nanoparticle based Drug Delivery System

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Abstract: Drug delivery systems (DDS) have advanced significantly in recent years, making it possible to provide medications more effectively. In order to develop DDS, biodegradable nanosized polymers underwent extensive investigation. In comparison to traditional drug delivery methods, nanoparticle (NP) based pharmaceutical administration offers a number of benefits, including biocompatibility, favorable pharmacokinetics, enhanced tissue macrophage distribution, higher permeability, and precise targeting. With continuous release of anti-tumor medications and better blood stability, NPs hold great potential for the treatment of cancer. Electrospun nanofibers have been created with mucoadhesive properties among others. The oral cavity is the mucosal region that has been examined the most since it is simple to work on and accessible.NPs can be directed to recognise cancerous cells and deliver medications precisely without harming healthy cells.Nano carriers are employed in cancer treatments to target the tumor cells via the carrier action of NP and positioning impact of the targeting chemical after absorption. The inclusion of nucleic acids and common chemotherapy agents inside the nano carriers indicates that NPs are used in both cytotoxic and gene therapy. Targeted nanoparticles for particular drug resistance pathways may result in improved multi-drug resistance reversal. Additionally, studies exploring the application of nanoparticles in immunotherapy have recently started. Nano delivery systems can address the benefits of effective targeting of a variety of distinct cell types. The promise for nanotechnology to enhance medical treatment for a life-saving strategy lies in precision therapy that avoids life-threatening adverse effects.

Keywords: Nanosized polymers; Nanoparticle; Electrospun; Mucoadhesive properties

Polyunsaturated fatty acids enhance the toxicity of doxorubicin on ovarian cancer.

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Abstract: Ovarian cancer is the most lethal gynaecological malignancy due to its poor diagnosis. A common chemotherapy drug used to treat many malignancies, including ovarian cancer, is doxorubicin (DOXO), which works as a DNA intercalator but also has some very prominent side effects, like drug resistance. It has been demonstrated that polyunsaturated fatty acids (PUFAs) have inhibitory effects on the development of ovarian cancer cells, but its combination studies with chemotherapeutic agent on ovarian cancer has not been explored very well. The present study shows that a combination of these PUFAs and a chemotherapeutic drug DOXO significantly increases the cytotoxic effect of the DOXO. The synergistic effect of DOXO+ PUFAs was found to be stronger than that of DOXO alone, which was evaluated by various anticancer assays.

Keywords: Ovarian cancer, Doxorubicin, drug resistance, polyunsaturated fatty acids, chemotherapy

Poster Presentations

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MIT School of Bioengineerig Sciences & Research
MIT Art, Design and Technology University, Pune

Production and Applications of Amylase: A Concise Review

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Abstract: Amylase is an extracellular enzyme that can be obtained from a variety of species, including yeast, microbes, and actinomycetes; however, the enzyme from fungus and bacterial sources has dominated recent usage in comparison to plant and animal source. Due to its vast applications in the baking, food, textile, and detergent industries, interest in the microbial production of the enzyme has risen considerably in recent years. In microorganisms, two primary types of amylases, α-amylase, and glucoamylase, have been found. In addition, a few microbial strains have also reported β-amylase, which is of plant origin. Typically, these amylases are extracellular and widely dispersed among bacteria, actinomycetes, and fungi. Interestingly, the first industrially made enzyme was an amylase. In this review, we want to conclude by recommending the use of microbial amylase due to its straightforward production process, low capital expenditure, low energy requirement, and high yield during production, as well as the exploration of additional microbes with the potential for producing enzymes and improved industrial scale production of the amylase for the improvement of the economy and industrial production of goods.

Keywords: Amylase; Starch; Bacillus; Fungus; Isolation

Hydrogel- based dressing in diabetic foot ulcer treatment

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Abstract: Diabetic foot ulcer (DFUs) is an open sore or wound that typically develops on the bottom of the foot and affects 15% of people with diabetes. Main vehicle for development of ulcers in diabetic population is poor circulation and peripheral neuropathy. This chronic injury frequently leads to non-traumatic lower leg amputations due to lack of wound healing. Wound healing is a process that heals or repair the affected sites by secreting multiple growth factors and cytokines at the wound site to heal the chronic wound, any changes that interfere with the healing processes can aggravate tissue damage and extend the repair time. Dressings become an essential component for ulcer treatment, it provides very good antibacterial coverage and help in managing wound infection. It comes in various form including hydrogel dressing. Hydrogels are three-dimensional network which can be fabricated from natural polymers and synthetic polymers. They have become increasingly attractive in biomedical science research, drug delivery and tissue engineering due to their tunability, versality and biocompatibility applications. This review provides a broad overview of recent development and innovation of hydrogel-based dressings which is more effective than the contact wound dressing in diabetic foot ulcer.

Keywords: Hydrogel; diabetic foot ulcer; infection; wound dressing.

In-Vitro evaluation of TiO_2 nanoparticles bio-synthesis from *Saccharomyces cerevisiae* conjugated with *Linum usitatissimum* gel for efficient treatment of wound healing in diabetic patients.

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Abstract: Diabetes Mellitus (DM) is a normal endocrine problem characterized by a range of high levels of glucose in the blood than the usual value (hyperglycemia). DM and its adverse effects cause the diabetic foot ulcer (DFU), DFU is co-ordinated with improper wound healing, because of ineffective cytokine and cellular response, poor vascularization, and neuropathy. The significant therapeutic methods for the management of improper wounds could be available via effective involvement of molecular mechanism and etiology of diabetic wound healing. Nanotherapeutics-based agents developed within the 1-100 nm range, which contain nanoparticles are the recent effective treatment strategy for improving wound healing in diabetic patients. Nanoparticles are smaller in size and have a large surface area that gives the biological interaction and helps for getting inside of the wound and performs the cell-cell communication, cell proliferation, vascularization for effective wound healing. The development of drugs that accelerate wound healing is a crucial subject. On account of that several herbs and plants like *Linum usitatissimum* (flaxseed) have been experimentally proved for efficient treatment of wound healing. The omega-3 fatty acid is the main precursor which is present in the flaxseed helps to improve wound healing by boosting the immune response. Hence the present study comprises the biosynthesis of Titanium dioxide (TiO2) nanoparticles (NPs) from *Saccharomyces cerevisiae*, preparation of flaxseed gel and conjugated with TiO2 NPs (TiO2 + FS gel) for evaluation of its ability in diabetic patients wound healing. The characterization of biologically synthesized TiO2 NPs was conducted by UV-Visible Spectrum (UV-Vis), X-Ray Diffraction (XRD), and Scanning Electron Microscope (SEM). The anti-bacterial activity of the TiO2 +FS gel was performed by the agar well diffusion method against selected pathogenic bacteria from the literature that is present in the wound. The hemolytic assay was performed on a test substance to identify whether it leads to breaking the erythrocyte cells. *In-vitro* and *In-vivo* analysis of the TiO2 + FS gel was performed by using the Wound Scratch Assay and HET-CAM test for

proving the test substance was anti-allergic. And finally, the mode of action of TiO2 + FS gel was identified by performing molecular docking using bioinformatic tools.

Key Words: Titanium dioxide nanoparticles, diabetic mellitus, wound healing, HET-CAM, *Linum usitatissimum*, X-ray diffraction, wound scratch assay, molecular docking, hemolytic assay, bioinformatic tools.

Sublimation of drugs from the site of application of topical products

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Abstract: The objective of the project was to investigate the plausibility of active pharmaceutical ingredients (APIs) to undergo sublimation from topical application following evaporation of solvent. Topical formulations with different APIs were subjected to sublimation screening test. The APIs in the selected topical products was found to undergo sublimation to a different extent. The salicylic acid topical product was found to undergo a significant loss due to sublimation. The extent of sublimation of salicylic acid was significantly greater at skin temperature compared to room temperature. When the APIs were subjected to the sublimation screening test in their neat form at $32\pm1^{O}C$, the natural log of the rate of sublimation decreased linearly with the standard enthalpy of sublimation of compound (R^2= 0.93). The formulation composition was found to have a significant impact on the extent of sublimation of the representative API, salicylic acid. The sublimation of API from the topical product was found to significantly affect the mass balance studies in case of the salicylic acid ointment. Furthermore, the results of the human studies agreed with the in vitro experimental results demonstrating the plausibility of loss of API due to sublimation form the site of application.

Keywords: Metamorphosis, solvent evaporation, secondary exposure, bioavailability, dermal penetration.

A comprehensive in-silico analysis of non-synonymous SNPs of human TSC2 gene

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Abstract: Tuberous sclerosis complex (TSC) is an autosomal dominant multisystem disorder in which cellular proliferation and differentiation are dysregulated, leading to the development of hamartomas in many organs, including the brain, skin, heart, kidneys, and lungs. A wide range of signs, symptoms, and complications are observed due to the unpredictability of the hamartoma distribution making a clinical diagnosis difficult. The role of TSC1 and TSC2 gene mutations is evident in TSC. TSC1 and TSC2 encode the proteins Harmatin and Tuberin respectively, which interact to form a complex that negatively regulates cell growth by inhibiting signal transduction by preventing p70 S6 kinase activation. The frequency of TSC cases caused by TSC2 gene mutations is consistently higher and associated with more severe disease complications. However, to date, functional significance for the majority of the TSC2 variants is yet to be elucidated. In the present study, we determine the potential functional consequences of nsSNPs of TSC2 by employing various computational approaches. Computational analysis to predict the possible structural and functional impact of nsSNPs on Tuberin protein was performed by different in *silico* tools. 68 SNPs out of 3204 were identified as deleterious with higher prediction accuracy. These SNPs were later subjected to stability and conservation analysis. 62 SNPs were predicted to be present in the highly conserved region (13 in TSC1 interacting region and 49 in RAP-GAP Domain of Tuberin) and 24 of them were revealed to cause decreased stability with a high confidence score. This study will assist in identifying potential targets for diagnoses and therapeutic interventions, especially if clinical and genetic analyses are inconclusive.

Keywords: Tuberous sclerosis complex, TSC2, Tuberin, in-*silico* analysis.

Parkinson's Disease Therapeutic Management: Drug Repurposing and Molecular Repositioning

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Abstract: Neurodegenerative diseases such as Parkinson's Disease are predominant in geriatric populations and an abject lack of therapeutic measures to cure the disease is desired. All current therapeutic management strategies aim at palliative care and alleviate symptoms. The disease is characterized by an imbalance in the Dopaminergic pathways. The formation of lesions in the Substantia Niagra pars compacta (SNpc) and the nigrostriatal tract. This results in a deficiency of dopamine (DA) in the striatum, which creates an imbalance between the dopaminergic and cholinergic systems resulting in motor defects such as – akathisia, dyskinesia, and involuntary tremors in the afflicted individuals. The primary choice of treatment is the dopamine analog L-DOPA, which however fails to sustain symptomatic care as the disease progresses to a stage of peripheral neuropathy. Conjunct therapy with MAO-B inhibitors, DOPA decarboxylase inhibitors, and (COMT) inhibitors is required to enhance the dopaminergic neuronal function. The efflux of the drugs from the BBB increases exponentially as the disease progresses, indicating a requirement for newer, more efficient drug analogs for better recovery in afflicted patients. The current study focuses on the development of newer analogs of the MAO-B and COMT Inhibitors by employing strategic repurposing and repositioning techniques and validating the antagonistic activity by performing Molecular Docking for 15 such analogs. The pharmacokinetic properties of the molecules were estimated by the structure read-across module using the SwissADME tool and safety profiles of the molecules were also predicted using decision-tree-based Tox-QSAR methods to assess the carcinogenic, mutagenic, and endocrine disruption potential.

Keywords: Parkinson's disease, dopamine, drug repositioning, molecular repositioning, and in silico analysis.

Isolation and screening of plant endophytic bacteria to control phytopathogens and plant growth promotion through volatile organic compounds

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Abstract: Bacteria produces and excretes a versatile array of volatile organic compounds (VOCs) with different biological activities. These VOCs reported for plant growth promotion and biocontrol ability against plants pathogens. In this study, plant endophytes have been isolated from tomato and screened for their biocontrol activity against plant pathogenic fungi such as *Rhizoctonia solani*, *Macrophomina phaseolina, Fusarium oxysporum, Magneporthe oryzae*, as well as against pathogenic bacteria such as *Xanthomonas oryzae* and *Pseudomonas syringae* through production of VOCs. Experiments were carried out on dual plates, where fungi were grown on potato dextrose agar (PDA) and isolates were grown on Luria bertani agar (LB) medium. LB media plates streaked with isolates first exposed to blank PDA plates for 3 days and after exposure, fungal bead placed on the exposed PDA plates and incubates at 28^0C for 2-3 days. Among all the VOCs producing endophytic isolates, five isolates TS6, PE4, TMG3, PE10, and L5 showed maximum biocontrol activity against targeted fungi. Isolates L5, PE4 and PN6 showed maximum biocontrol activity against *Xanthomonas oryzae* when grown on a same plate. Isolates were further, screened for their PGPR activities such as siderophore production, P solubilisation, KOH test, catalase test and PE10 and TMG3 showed maximum siderophore activity while PE10 and PE4 showed P solubilisation activity. These results showed that VOCs might help in prevention of plant diseases, promote plant growth and used as biocontrol agent alternate to agrochemicals and additive towards sustainable agriculture.

Keywords: Volatile organic compounds, antifungal, antibacterial, plant growth.

Semipermeable polymer Coated microneedles for prolonged drug delivery

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Abstract: Microneedle (ML) arrays consists of micrometersize needle like projections which are used for overcoming the tissue barrier and deliver active pharmaceuticals. The drug was in the core ML which was coated with a semipermeable polymer. Hence, controlled release of only the API (and not the excipients) is possible unlike uncoated polymer. Prolonged delivery is relatively more safer and pharamacologically beneficial particularly when delivered inot the sensitive tissues, compared to immediate delivery of drugs. The potential application of semipermeable layer containing MLs in dermal and transscleral drug delivery was explored using excised porcine tissue modes. The MLs were formulated with 50%w/v PVP K30 and it was coated with 4%w/v ethyl cellulose or 1.5%w/v Eudragit E100 by an optimized coating process. The prolonged release of lidocaine (ethyl cellulose coated), and 5-Fluorouracil (5-FU) (Eudragit E100 coated) was investigated for dermal delivery. Likewise, the prolonged delivery of voriconazole and dexamethasone was investigated for tran-sclearal delivery into the vitreous humor. Microscopic studies revealed that the coating remained intact even after exposure to tissue fluid. Thy complied with the stability required when subjected to stress conditions.

Keywords: Controlled drug delivery, melanoma, cancer, topical, melanocytes, ocular, vitreous humor, dissolvable microneedles.

In silico approach for pathway reconstruction to unravel the evolutionary significance of cannabinoid biosynthesis

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Abstract: Cannabinoids are naturally occurring bioactive compounds found in several plant species other than *Cannabis sativa* that exhibits drug-like effects throughout the body, including the central nervous system and the immune system. The major phytocannabinoids are tetrahydrocannabinol (THC) and cannabidiol (CBD) which are extracted for treating conditions like anxiety, chronic pain, and nausea. The legal policies impose major challenge in perusing research to utilize the compound for medicinal purpose; therefore, an attempt has been taken into consideration to develop an insight for the cannabinoids' biosynthetic pathways. On reconstructing the biosynthesis pathway of cannabinoids it was found that cannabinoid production proceeds from pyruvate which in turn is a product of glycolysis. The pathway represents a descriptive topology of network metabolites and enzymes yielding important information on their evolution. The gap in the evolution and phylogenetic relationships of the enzymes involved in cannabinoid biosynthesis remains unclear. They are majorly incorporated in the prenylation, and cyclization of the reaction intermediates along with the decarboxylation of the cannabinoic acids resulting in the production of both the major and minor phytocannabinoids. Using the pathway reconstruction strategies we have studied not only the co-evolution of the biosynthesis pathway but also the understanding of the ancestral relationships among the enzymatic proteins involved.

Keywords: biosynthesis, cannabidiol, tetrahydrocannabinol, pathway, phylogeny, phytocannabinoid.

Isolation and Identification of microbial species from agricultural land with herbicides 2,4-D and MCPA

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Abstract: Regular use of herbicides worldwide in agriculture are phenoxyalkanoic acid herbicides, which belongs to various plant hormones are kind of xenobiotic herbicides. Use of phenoxyalkanoic acid herbicides in agricultural and non-agricultural areas is regularly used, mainly 2,4-D (2,4-dichlorophenoxyacetic acid) and MCPA (4-chloro-2-methylphenoxy- acetic acid) and their derivatives. However, their use is quite beneficial but their long persistence in environment for long time have detrimental impact on natural soil and its fertility. These herbicides are highly effective against annual and perennial broadleaf weeds in cereals, corn, sugarcane. Microorganisms are utilized in bioremediation for the detoxification and degradation of pollutants. There has been increased attention given to this technology since it has shown to be both effective and reliable in removing pesticides from polluted environments. In present study, soil sample is collected from agricultural land where regular use of these herbicides is done. Microbial organism isolated from the samples in presence of herbicides at concentration lower than recommendation dose on field separately. Pure culture species is isolated separately in presence of both the herbicides, identification and characterization is being performed for all the isolated strains based on their plate morphology, gram staining and shape under microscope. Further identification based on the 16s DNA is under process.

Numerical and experimental investigation of the influence of tumour parameters on surface temperature

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Abstract. Breast cancer is the leading cause of cancer-related deaths among women. The timely and early diagnosis of the disease is the only way to regulate this type of cancer. Thermography is a type of non-invasive imaging technique that makes use of temperature distribution on the breast surface to detect the presence of a tumour. The major purpose of this research is to analyse the influence of tumour depth and size on surface temperature via simulation and experimental method and drawbacks of thermography for breast cancer detection. A computational study had been carried out for a tumour of sizes $4.17cm^2$, $3.14cm^2$ and $2.01cm^2$ and corresponding temperature difference on the surface were obtained. Likewise, the depth of the tumour was varied from 0.5 *cm* to 3 *cm* from the surface and temperature changes were plotted. The experimental analysis was done with a silicone phantom embedded with electrical resistance to replicate internal heat generation due to the tumour. Temperature measurement was done using a thermocouple. The steady-state temperature of the tumour in different depths and size were executed. Current simulation and experimental evidences suggest that tumour located deeper and smaller in size provides only less hot-spot temperature. In such a situation the tumour tissue has to be thermally energized independently, to increase the thermal contrast on the surface.

Keywords: Active thermography, Breast cancer, Thermal imaging, Thermography, Non-Invasive imaging, Pennes Bioheat equation.

Stepping stones of motion intention prediction

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Abstract: Motion Intention Prediction is prediction of the next action performed by the person based on the EMG signals. Its applications range from rehabilitative, industrial and defence. The aim of conducting the study is to aid the soldiers with exoskeletons they are in control off, which will assist them increase their performance. Active exoskeletons have proven their reliance in terms of reducing the load which can be seen through decreased muscle activation, metabolic activity, pressure in the FSR insoles. To act as master, exoskeleton has to recognize a future phase which is going to occur for a subject in order to avoid resistance to the intended activity. Electromotive Delay [EMD] is the delay between the initiation of the actual motion and the detection of EMG onset in muscles. It's reported to be in the range of 30-100 ms varying with respect to muscles in consideration. In this poster, EMD has been studied for lower body superficial muscles for 10 subjects using EMG and accelerometer signals. EMD was found to be between 60-70 ms for gastrocnemius, tibialis anterior, vastus lateralis and medialis and rectus femoris and between 20-60 ms for sartorius and semitendinosus.

The aim of this study is to predict stance and swing phases of a GAIT cycle exploiting the electromechanical delay, which will further pave the path for much more complicated predictions such as, predicting all of the phase of GAIT cycle, classification of various activities, classification of activities with load being carried and finally predict the motion itself.

Keyword: Motion intention prediction, electromechanical delay, muscle activations, GAIT Cycle, classification.

A new antibacterial bioactive glass for bone tissue engineering: an *in vitro* study

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Abstract: The usage of bioactive materials in clinical application has been extensively increasing day by day as they serve as an implant to heal or to compensate for bone loss or damage. The use of various glass systems by taking advantage of trace metal ions for their biomedical applications is indeed increasing research and development activities. This study presents the effect of addition of Chromium (Cr) on structural and in vitro biological properties of optimized bismuth borate glass. The bismuth borate glasses containing Cr_2O_3 have been prepared by melt-quenching method. Physical, structural and *in vitro* biological properties were evaluated. Bioactivity was examined *in vitro* by immersing glass powders in simulated body fluid (SBF). E. Coli and S. aureus bacterial microbes were used to test antibacterial activity of glasses by disc diffusion method. Cytocompatibility was analyzed at different concentrations using Osteosarcoma cell line by MTT assay. The results show that the increase in density, and decrease in molar volume of glasses with increasing Cr_2O_3 concentration. *In vitro* bioactivity study demonstrated good hydroxyapatite formation rate on the surface of glass samples with increase in pH of SBF solution, Cr_2O_3 concentration up to 0.3 mol.%, but higher concentration of Cr_2O_3 inhibited the formation of hydroxyapatite layer. All the Cr doped glasses showed bactericidal effect against E. Coli and S. aureus as well as cytocompatibility with MG 63 cells

Keywords: Bioactive glass, antibacterial activity, bone tissue engineering, bismuth.

Impact of hexaconazole residue on the grape metabolome and identification of potential biomarker metabolites

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Abstract: In viticulture, seasonal pests and diseases are controlled by different pesticides application. Besides their application, pesticide residue is found to affect the plant's metabolite profile and ultimately hamper the product quality. Hexaconazole (HX) is a systemic triazole fungicide used to control fungi in grape. The present work was undertaken to study the dissipation of hexaconazole in the wine grape variety Cabernet Sauvignon and to explore the impact of its residues on the grape metabolome.

Hexaconazole formulation was applied at the recommended dose (HX-RD) and 10 times SD (HX-10 RD). The pesticide dissipation kinetics was studied by extracting the samples with QuEChERS. The berry samples were analysed by LC-MS/MS. The dissipation study showed 0.057 mg kg−1 IM residue for SD at the time of harvest. The HX-SD and HX-10RD showed 93% and 80% dissipation from 0 to harvest days, respectively.

The biochemical analysis of grape berries at harvest revealed a clear distinction between HX-SD and HX-10 RD. In HX-SD and HX-10 RD treated berries, the flavonoid content was increased to 42% and 99%, respectively as compared to the control sample. In contrast, phenols and antioxidant capacity were decreased by 73.34% and 21% in HX-10RD. The anthocyanin content was reduced to 50 and 52.42% in both treatments.

The non-targeted analysis of berries revealed the variation in metabolites. The differential expression of metabolites indicated that the HX drastically affected the metabolome. In total, 26 metabolites in HX-SD and 21 metabolites at 10RD showed significant variation (adj. p values <0.05).

In this study, biomarkers for HX residue were identified. The compounds in HX-10RD viz., 4-Guanidinobutanal, 2-(N-HEPTANOYL) THIOPHENE, DL-Arginine, DL-Arginine were identified as biomarkers (log2 fold≥1, adj p-value ≤0.01). In HX-SD treatment, biomarkers Isorhapontigenin, Piceatannol, 4-Methylene-L-glutamine, DL-Arginine, Homoarginine were identified. The metabolite of hexaconazole i.e. 2-Isopropyl-5-thieno [3,2-b]thiophen-2-yl-1,3,4-oxadiazole is commonly found as a biomarker in both cases. It could be a potential biomarker for identifying and authenticating organic produce for HX residue.

The study gives an insight on the impact of hexaconazole residues on grape global metabolome, and biomarker identification would be useful in future for food safety evaluation.

Keywords: Hexaconazole, metabolome, biomarker.

Structural characterization and *in vitro* bioactive assessment of with and without gallium-doped bioactive glasses

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Abstract: Bioactive glass nanoparticles with and without Ga_2O_3 (named Ga-MBG and MBG respectively) were synthesized through the emulsion-assisted sol-gel method and characterized by FT-IR, XRD, and FE-SEM with EDX. The XRD confirmed the amorphous nature of the respective glasses after stabilization. The FE-SEM revealed that the roughened surfaces had a spherical shape. The Zeta particle size distribution revealed that particles with average diameters of 200 nm are slightly larger than those measured by FE-SEM (150 nm). Finally, the zeta potential of bioactive glass nanoparticles suspended in tris buffer solutions at various pH levels and also in deionized water was determined. The bioactivity of these materials was determined in vitro by examining the ability of apatite to form on the surface after immersion in simulated body fluid (SBF). The pH variations, XRD, and FT-IR results were used to confirm the materials' bioactivity, and also calculate the Ca/P ratios to confirm the surface changes using FE-SEM with EDX analysis. Finally, all samples had a bioactivity property which could demonstrate their ability to treat bone regeneration.

Keywords: Silicate bioactive glass, hydroxy apatite layer, gallium oxide.

Nicotine metabolite as a ligand in hydrothermal synthesis of Cobalt superstructures

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Abstract: The substantial growth in the field of environmental pollution assessment and control has triggered the need of unique and newest approaches. The implication of various kind nanomaterials to scavenge the pollutants from environment is a multifaceted avenue for the researchers. In this context various magnetic metal superstructures are playing vital role due to their ease of synthesis and employment along with flawless operation and recyclability. In the present study, magnetic cobalt flower like superstructures were synthesized by facile hydrothermal method. A nicotine metabolite obtained from bacterial biotransformation by *Paenarthrobacter sp*. was used as a ligand in the formation of cobalt superstructure with cobalt chloride. The role of ligand in superstructure formation was studied by altering its ratio in the reaction and the resulted optimum ratio showed the formation of a floral superstructure by mutually arranged fern like petals. The nucleation and assemblage process were observed by keeping sodium acetate as control ligand. The tested ligand exhibited entirely different morphology compared to control. The material so obtained was further analysed by FE-SEM, EDS, FTIR, XRD, and magnetometry. These superstructures then employed in removal of environmental pollutants.

Keyword: Magnetic, superstructure, nicotine metabolite, ligand, FE-SEM.

Spinal Cord Fracture Interpretation by 3D Channel-Separated Convolutional Networks with Model Segmentation and Classification Utilizing Saliency Maps.

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Abstract: Over the past ten years, Convolutional Neural Network (CNN) models have achieved notable progress in resolving difficult vision problems. However, these deep models are regarded as "black box" methods since it is difficult to fully comprehend how they operate at the fundamental level. This research is an attempt to move toward explainable deep learning models, which have recently received a lot of attention. Grad-CAM++, an expanded variation of the newly proposed Grad-CAM approach, in comparison to the state-of-the-art. Grad-CAM++ is able to better visualize predictions made by the CNN model, both in terms of better object localization and the explanation of the occurrence of many instances of the same object in a single image. By combining the positive partial derivatives of the final convolutional layer feature maps with respect to a specified class score, the proposed method, which generates a visual explanation for the associated class label, is justified mathematically. Grad-CAM++ offers promising visual explanations for a specific CNN architecture that are human-interpretable for a variety of tasks, including classification, creating image captions, and recognizing 3D actions, as well as in novel contexts like knowledge distillation, according to our extensive tests and evaluations—both subjective and objective—on common datasets. Prior to Grad-CAM++, we employed a saliency map technique. Saliency maps are a technique for visualizing a neural network's decision-making p process. They aid in understanding the primary objectives of each convolutional layer as well. This makes it a little bit easier for us to comprehend how decisions are made. Saliency maps allow us to see the areas of a prediction that the convolutional neural network is paying particular attention to. Bounding boxes were used to visualize the data by being drawn around the locations of interest. The following format is used to draw the bounding boxes on the photos using the coordinates from the heatmap: (width, height, x centre, y

centre). Therefore, Model was segmented, classified and visualized based on Convolutional Networks.

Keywords: Convolutional Neural Network (CNN), Grad-CAM++, aliency map, Bounding boxes, Segmentation, Classification, Visualization.

Anticancer activity of curry leaves extract

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Abstract: Ovarian cancer is the most lethal gynecological cancer, due to its late diagnosis. The incidences of ovarian cancer in India are increasing at an alarming rate. OC is mostly diagnosed between 55-60 years of age. While OC has worst prognosis with 5-year survival rate. Drug resistance developed at later stages further decreases survival rates in ovarian cancer patients. Natural compounds isolated from plant extract can have promising potential in cancer treatment due to their minimal side effects. Curry leaves are commonly used in Indian cuisines, and are known to have antimicrobial, antifungal, and antioxidant activity. However, very few studies show the effect of curry leaves extracts on cancers, especially ovarian cancer. This study has screened various extracts of curry leaves for antimicrobial and antifungal activities and were tested for cytotoxic effects on ovarian cancer cell line – PA1 by MTT assay and Annexin V-PI staining, wherein the extracts showed significant anticancer activity via apoptosis pathway. Extracts also showed to have antiangiogenic effect with no teratogenic effect on chick embryos [HH stage 26 (120h+)]. This suggest that such extracts can be a potential therapeutic option against ovarian cancer. However, in depth studies will be carried out to understand mechanism of action which will help us to harness its maximum potential.

Keywords: Curry leaves, plant extracts, ovarian cancer, anticancer activity, angiogenesis, apoptosis, CAM assay.

Biopolymer assisted synthesis of metal oxide nanoparticles for catalytic and biological application.

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Abstract: The applications of copper nanoparticles in the fields of biological, physical, and chemical sciences are extremely diverse. These nanoparticles made from natural extracts are getting more and more prominent in the fields of nanotechnology and green chemistry since the greener the approach, the better the product. Here copper oxide nanoparticles (CuO-NPs) are produced biochemically by galactomannan extracted from *Ceratonia siliqua*. Powder X-ray diffraction (XRD), ultraviolet-visible spectroscopy (UV-Vis), field emission scanning electron microscopy (FE-SEM), and Fourier transform infrared spectroscopy (FTIR) techniques were used to investigate CuO-NPs. CuO-NPs synthesized using galactomannan had a high absorption peak in the UV-visible spectrum. The development of polycrystalline structures with typical grain sizes between 13.7 and 19.5nm was confirmed by XRD investigation. The stretching vibrations of -O-H, C-H, C-N and C = O groups with various functional groups involved in the reduction and stability of nanoparticles were detected in FTIR spectra. The current study sheds insight into the biological (antimicrobial, anti-cancerous) uses of CuO-NPs and their photocatalytic activity. The nanoparticles displayed a minimum inhibitory activity of 51% inhibition at concentrations of 500ug/ml of 0.25-NP against E.coli. We report 99% inhibition of *E. coli* using Biofilm assay for 1.00-NP. The goal of the current work is to describe an efficient, comprehensible, and environmentally friendly process (sometimes referred to as a "green method" or "green chemistry") for producing CuO-NPs and to assess its potential for use in a range of commercial and clinical applications.

Keywords: CuO Nanoparticles, Green synthesis, Biochemical Assays, Photocatalysis

Synthesis and characterization of Biocompatible Chitosan Coated Zinc Oxide Nanoparticles and it's In vitro Cytotoxicity studies on MCF-7 and MCF-10A Cell lines

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Abstract: Nanoparticles of zinc oxide (ZnONPs) are known for their antimicrobial and anticancer properties. Owing to their high surface charge and small size, ZnONPs show high cytotoxicity which is a major issue. In order to make ZnONPs more stable and biocompatible, they need to be coated with a biocompatible agent. Chitosan (CS) is a cationic biocompatible biopolymer used for stabilizing nanoparticles. In the current study, a simple chemical precipitation method was used to synthesize bare ZnONPs and CS coated ZnONPs (CS-ZnONPs). The nanoparticles were characterized using UV-Vis spectrometry, FTIR, XRD, Zeta potential, DLS, ICP-AES and TEM. MTT assay was used to examine the cytotoxicity of the synthesized system on MCF-10A and MCF-7 cells in-vitro. Acridine orange/Ethidium bromide (AO/EB) staining was used to study morphological changes in cells post treatment. Hemolysis studies were conducted using human RBCs to understand the biocompatibility of the above nanosystems. Characterization data confirmed the successful synthesis of biocompatible CS-ZnONPs in the desired size range. In vitro data suggest higher cytotoxicity against breast cancer cell line MCF-7 compared to normal human breast epithelial cell line MCF-10A. Also, AO/EB staining showed visible signs of apoptosis in MCF-7 cells post treatment. The hemolysis assay performed confirmed that CS-ZnONPs did not cause haemolysis upon interactions with RBCs thereby proving their biocompatible nature. Above results support the anticancer potential of CS-ZnONPs towards MCF-7 breast cancer cell line.

Keywords: ZnONPs, chitosan, MCF-7, MCF-10A, biocompatible, breast cancer.

Synthesis of Activated carbon from Plastic waste

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Abstract: The primary cause of pollution in the air, water, soil, and oceans is considered to be plastic waste. It has a non-dissociation feature and is not biodegradable. Over the years, plastic has contributed to raising the worldwide living standard. Plastic is a bad choice for the environment because of the unpredictability and unplanned end of life management. A significant amount of the waste produced globally is made up of polymers from plastic trash, including polypropylene, polyethylene, and polyethylene terephthalate, etc. Researchers have been seeking for alternative solutions to the issues caused by such significant amounts of waste plastic for many years.

To reduce the amount of plastics produced, the carbon from plastic waste using the pyrolysis approach was synthesized. The catalyst, which is essential for the preparation of carbon material, in this study Nickel, Iron along with their sulphates & nitrates and Citric Acid was used as a catalyst for carbon synthesis. The temperature of the synthesis process was reduced to 500–600 ^{0}C, at atmospheric pressure in simple device of Muffle Furnace. Further, the obtained samples were characterized by FTIR and SEM.

Keywords: Plastic waste, FTIR, SEM, synthesis, activated carbon

Doxorubicin loaded biopolymeric n-PUFA lipid nanoparticles for anticancer applications.

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Abstract: The current study aims to develop Doxorubicin loaded biopolymeric lipid nanoparticles for anticancer applications. The conventional drug delivery system faces multiple challenges in terms of its efficacy and tunability. Also, the uncontrolled drug delivery profile makes it difficult to have control over the required dosage administration. The chemically synthesised systems also have the immense challenge of toxicity when administered. This work was aimed to synthesize biopolymeric nano-conjugates in combination with drug Doxorubicin and n-3 PUFA. Omega-3 polyunsaturated fatty acid (PUFAs), in combination with doxorubicin enhances the antitumor activity of chemotherapeutics. It is hypothesized that this combination increases the antitumor efficacy as n-3 PUFA promotes oxidative stress and subsequent lipid peroxidation of tumor cells which makes it a better combination than lipodox treatments. Also, Doxorubicin as the model drug is used to evaluate its drug delivery profile and comparative cytotoxicity assays. The result showed that the prepared stable & mono dispersed nano-conjugates were successfully adsorbed with the drug Doxorubicin. The release profile projected a duration of 8 hours with a moderate drug release. Cell Viability and proliferation were analysed using MTT Assay and Scratch Assay by treating the PA-1 ovarian cancer cell line with drug loaded nanoparticles. Various characterization studies like UV Spectroscopy, FTIR and analysis of Bioassays indicates immense potential of this chemotherapeutic combination to be used in various healthcare applications as a smart drug delivery system.

Keywords- Doxorubicin, Biopolymeric Nano-conjugates, Bioassays, Smart Drug Delivery.

Development of Biopolymeric antimicrobial nanomaterial-based bioplastic for biomedical applications

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Abstract: This study aimed to develop biopolymeric antimicrobial nanomaterial-based bioplastic for a wide range of applications. Healthcare and the biomedical industry use an ample amount of synthetic materials prepared from chemical constituents for adhesive coatings, packaging items, scaffolding materials etc., facing challenges of toxicity, biocompatibility and non-tunable properties. The current work helped in developing a biopolymeric silver conjugated nanomaterial based bioplastic that can replace the chemically synthesized ones. The prepared product showed improved properties like increased tensile strength, hydrophobicity, antimicrobial properties against gram-negative as well as gram-positive bacteria. The application of these prepared nanomaterials is widespread in the biomedical and healthcare industry as base material having the least toxicity, increased biocompatibility and tunability in terms of tensile strength, thickness and related physical properties.

Keywords: Nanomaterial, biomedical, antimicrobial, nanoconjugate.

User authentication system using Gait analysis

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Abstract: A gait analysis is a well-established tool for the quantitative assessment of gait disturbances providing functional diagnosis, assessment for treatment planning, and monitoring of disease. A gait pattern can be potentially used as a signature for user authentication. The aim of this work is to develop a user authentication system using gait analysis. A publicly available gait dataset in which 4 walking sessions of 93 subjects were recorded by two smartphones placed on the left waist & right thigh is used to characterise the walking person or user. We emphasised on distinctive biometric features such as accelerometer data and gyroscope data of the user. The data is pre-processed using normalization, outlier removal and principal component analysis to extract the features. The features are used by ensemble based Random Forest models to obtain distinctive gait patterns and authenticate a user. The model is optimized using GridSearchCV for number of trees, depth of the tree and number of gait instances features. It is found that the proposed methodology has outperformed the existing methods for user authentication using gait analysis. Further, the proposed methodology can be useful to identify daily activities of a user and purpose of monitoring activities of elderly persons.

Keywords: Gait Analysis, Functional diagnosis, Machine learning, User authetication, Random Forest, Principal Component analysis, GridSearchCV

Identification of Zinc (Zn^{2+}) degrading genes in bacteria through comparative genomics

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Abstract: Heavy metals are defined as metals that possess high densities, atomic weights or atomic numbers. These metals are considered systemic toxicants that are known to induce multiple organ damage, even at lower exposure levels. Some examples of heavy metals are Zinc (Zn^{2+}), Magnesium (Mg^{2+}), Cadmium (Cd^{2+}). Certain microorganisms play a significant role in the removal of heavy metal pollutants in rivers, seas, ocean and water bodies. The objective of this project is identification of Zinc degrading genes from bacteria. Genes can be enhanced and introduced to native strains to prevent toxicity.
The basic criteria for bacteria selection was its non-pathogenic characteristics. The bacteria chosen are *Synechococcus elongatus PCC 6301*, *Thiobacillus ferrooxidans* and *Bacillus safensis U41*. Gene identification is carried out by performing a comparative analysis of bacteria which elucidates gene information about the bacteria. Comparative analysis is performed using BioCyc webtool. Gene Analysis was done with regard to UniProt. The genes degrading specific metal Zinc is manually curated. Further, circular plots are generated via KBase and RAST analysis of genes connected to subsystems plot is generated.

Identified genes can be utilized by cloning Zinc degrading genes into bacteria that lack Zinc degrading properties. Thus, water bodies can be effectively and efficiently be cleansed of Zinc pollution.

Keywords:, *Synechococcus elongatus PCC 6301, Thiobacillus ferrooxidans, Bacillus safensis U41, Zinc (Zn^{2+}),* RAST and BioCyc.

Molecular Docking and Dynamics Studies of CDK1 against Epithelial Ovarian Cancer Drugs

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Abstract. Epithelial ovarian cancer has been researched to be the most common and aggressive form of cancer. Owing to its ability to evade detection until stage 3, when cancer has metastasized extensively, it is important and crucial to find an effective treatment. Keeping this concept in mind, we implemented *in-silico* analyses in the form of molecular docking and dynamics.

The gene CDK1, the encoder of the protein that is a member of the Ser/Thr protein kinase family. It is a catalytic subunit of the M-phase promoting factor (MPF), and a key player in the eukaryotic cell cycle. CDK1 plays a major role in cancer diseases and needs to use appropriate drugs against CDK1 protein to treat cancer. Our insilico studies on FDA drugs like imipramine, trazodone, propafenone, resveratrol, alpha estradiol, levonorgestrel, doxazosin, apigenine, rottlerin, nortriptyline, prochlorprazine, noretynodrel, chlomipramine, fluphenazine, amiodarone, medrysone, piperlongumine, daunorubicin, vironostat, methotrexate and scriptaid considered for molecular docking to know the better drugs among them. The active sites of the protein were analyzed using PDBSUM, and their neighboring amino acids were evaluated. The amino acids were observed to be Tyr 15A, Glu 81, Ile 10A and Leu 83A. The grid was calculated based on the coordinates of isoleucine, glutamine and tyrosine residues Grid formation was done based on the active site, and molecular docking was carried out using AutoDock Vina. The highest docking score observed was the protein against Doxazosin, showing a binding affinity of -10.4 kcal/mol. The interactions within the complex were observed using ProteinsPlus and Discovery Studio. Further, hydrogen bond, pi-pi interactions were noticed among the drugs with side chains of CDK1 protein of Thr 14A, Asp 128A and Asn 133A. Lys 130A showed pi-pi bond interactions with the ligand's aromatic rings. Our studies reveal that Doxazocin has the highest potential to treat epithelial ovarian cancer.

Keywords: Epithelial ovarian cancer, molecular docking, CDK1, doxazosin

Design and development of molecular network of differential gene expression of ovarian cancer

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Abstract: Ovarian cancer contributes to a significant number of deaths worldwide, with over 313,000 cases annually and mortality of about 200,000. More than 80% of women, predominantly of older age groups are diagnosed at advanced stages (stage III and IV), leading to less than 30% survival rate. At the advanced stage, therapies become increasingly ineffective due to drug resistance in cancer cells, raising an urgent need to develop new therapeutic strategies. In this study we investigated different datasets of ovarian cancer and an appropriate dataset was chosen (PRJNA782974). Further using Galaxy Server, RNA Sequencing Analysis was done to get the list of upregulated and downregulated genes. Gprofiler was utilized to gather more data regarding gene functions as well as in various metabolic pathways and processes. The molecular network was constructed with Cytoscape and the STRING database with confidence score of 0.4. Further, analyzed various gene clusters with degree of nodes, pathlegth, and betweenness among them with Network Analyst tool. These would be provide the identification of vital genes involved in treating ovarian cancer patients as well as scope to design and development of new drugs.

Keywords: RNA Sequencing Analysis, majorly expressed genes, Network interaction, Galaxy Server, Gprofiler, Cytoscape, String database, Network Analyst

Polyphenolic compounds extraction from *Cosmos sulpheheureus*: Potential Against Multidrug-Resistant Bacteria

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Abstract: In current scenario, a serious threat to human health is advent of extensive use of antibiotics that leads to emergence of multidrug-resistant (MDR) bacterial strain. It is also imposing a serious hurdle to the progression of drug discovery programs. Resent research is indicating the importance of plant secondary metabolites/phytochemicals in contending the drug-resistant strains. Different phytochemicals such viz. alkaloids, phenols, terpenes alone or in combination have been successfully demonstrated their inhibitory potential against different pathogens. Therefore, by considering the issue of multidrug resistance to pathogens, the present study designed to explore the potential of polyphenolic compounds extracted from *Cosmos sulpheheureus* leaves and flowers in combating antibiotic resistance and the resistant microbial pathogens by different combinations.

Keywords: *Cosmos sulpheheureus*, polyphenolic compounds, secondary metabolites, phytochemicals, multidrug-resistant bacteria.

Study of differential expression of genes in ovarian cancer using *in silico* methods

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Abstract: Ovarian cancer detection and diagnosis has been prominent challenges faced in the recent days. Treatment for the same is challenging because of the hurdles faced in the detection of the disease itself. Among all the gynaecological cancers, ovarian cancer is studied in depth. The genes predominantly associated with ovarian cancer are PRKN, CDH1, AKT1, ERBB2, OPCML to name a few. RNA-Seq analysis is performed using *in silico* methods (R programming language) on the sample datasets retrieved from NCBI-GEO. The microarray clinical samples were retrieved from the NCBI database which were then run by R programming language to find out the top differentially expressed genes using package like BiocManager and libraries like limma, pheatmap, GEOquery, ggplot to name a few. The differentially expressed genes were successfully retrieved from the imported clinical sample along with visualisation in the form of heatmaps and box plot.

Keywords: Ovarian cancer, RNA-Seq analysis, Differential gene expression, *In silico* methods

Unfolded protein response genes as novel biomarker in ovarian cancer – a proposal

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Abstract: Ovarian cancer is the 5th leading gynaecological malignancy based on the incidence rate, with the poor prognosis and high mortality rate among women across the world. The relative rate of 5-year survival for this cancer is 49%, mostly due to late stage diagnosis. CA125, the biomarker used for the diagnosis currently, is not a highly specific or sensitive one. Hence, researchers are working towards discovery of novel biomarkers for the diagnosis and prognosis of the disease. As cancerous cell has high proliferation rate, it requires increased activities of Endoplasmic Reticulum(ER) machinery for protein folding and processing. Cancer cells frequently encounters extrinsic stresses such as hypoxia, glucose deprivation, calcium depletion and growth factor withdrawal, these can perturb protein folding in ER and subsequently causes accumulation of unfolded or misfolded proteins in the ER, known as ER stress. Accumulation of unfolded proteins triggers a dynamic signalling network known as unfolded protein response(UPR), it primarily functions to restore protein homeostasis in ER or can activates apoptosis if protein homeostasis is not restored, depends on the level of ER stress. UPR is activated by ER stress and plays an important role in the tumorigenesis of ovarian cancer. However, the relationship between UPR genes and prognosis of ovarian cancer has not been studied widely. Here, we hypothesize that a molecular signature of genes involved in unfolded protein response pathway can be explored as novel biomarkers for early diagnosis and better prognosis of Ovarian cancer.

Computational analysis of microarray data for ovarian cancer

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Abstract: According to American cancer society, the year 2022 has seen 19,880 being diagnosed with ovarian cancer and 12,810 deaths due to this disease. The higher rate of death is due to delay in diagnosis of the disease. Early diagnosis and timely intervention increases the overall survival rate. However, the disease does not exhibit any specific symptoms, thus posing a challenge to the diagnosis. Transvaginal ultrasound and estimation of CA125 levels are the current diagnosis techniques. Several literature reports have posed questions on the specificity and sensitivity of these methods. Thus, appropriate diagnosis remains a challenge and has been the focus of researchers. Studies on gene expression based on microarray have been carried out by several researchers and these data are available on the NCBI GEO database In this study we analysed the microarray data available in the database using computational method to identify the differential gene expression. The datasets were classified based on their clinical features into Recurrent and non-recurrent tumours, early and late stage tumours, Primary and metastatic tumours, primary and ascitic tumours, and metastatic and ascitic tumours. The pathway analysis was performed for these genes and the hub genes were identified. Further analysis and validation using in vitro techniques may bring us one step closer to identifying novel biomarkers.

Drug Repurposing of FDA-approved kinase inhibitors for MRSA

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Abstract: In the new global economy, Antimicrobial Resistance (AMR) has become a central issue for physicians, patients and society as a whole. By 2050 AMR is predicted to be a leading cause of death, greater than cancer, diabetes and infectious diseases. Growing concerns of the practitioners have imbibed a sense of urgency among researchers, this led our group to tackle this crisis. Our group targeted three different types of resistance mechanisms (Gene modification, efflux Pumps and Surface protein A). The leading cause of AMR is by a drug resistant bacteria named Methicillin-Resistant Staphylococcus aureus (MRSA), which are basically, antistaphylococcal penicillins resistant strains of S.aureus. We targeted this due to growing infections of the bacteria in the hospital community. We tested its mechanism in the silico approach using Molecular docking studies and molecular dynamic studies using FDA approved Kinase inhibitors. These FDA approved drugs were repurposed for MRSA by global docking followed by local docking and further screening. Five drugs namely Tepotinib, Tucatinib, Radotinib, Capmatinib and Netrasudil, showed promising results as kinase inhibitors for repurposing against MRSA.

Keywords: Amr, MRSA, molecular docking, molecular dynamics.

Computational analysis of gastric cancer omics data using text mining

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Abstract: One of the most lethal cancers is gastric cancer, which develops as a malignant tumor in the mucosa, the lining of the stomach, and spreads through further layers. Early-stage diagnosis of gastric cancer is highly challenging because the patients either exhibit symptoms similar to stomach infections or show no signs at all. The biological molecules known as biomarkers are active players in the cancer process and act as indications of aberrant alterations brought on by malignant activity. Though there have been significant advancements in the biomarkers and therapeutic targets related to gastric cancer for detecting and treating the disease, there is still insufficient data to fully eradicate the disease in its early and late phases. Therefore, it is crucial for the healthcare industry to identify particular biomarkers for the detection and treatment of stomach cancer. The objective of this research work is data analysis in gastric cancer by employing computational techniques such as text mining, network analysis, next-generation technologies (NGS), machine learning (ML), deep learning (DL), and structural bioinformatics in order to identify biomarkers. The categorization of people with cancer and the identification of genetic markers in cancer and their subtypes are made possible by integrating data from multiple computational methodologies. A huge gene-drug interaction network will be analyzed in the current study, to forecast putative biomarker genes.

Building network of Virus-Molecule Association from Literature (ViMAL)

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Abstract: Viral diseases and viruses have long been of interest to the scientific community, particularly virologists. However, after COVID 19, it has gained the attention of everyone. Although significant progress has been made in this area, considerable work still needs to be done due to the unstructured distribution of the data. The approach reported here is a small effort to speed up progress by compiling scattered data. In order to investigate the relationship between viruses and their molecular affiliations cited in the literature published in the previous 50 years, the study primarily entails the establishment and development of a database named ViMAL (Virus-Molecule Association from Literature). Additionally, chemoinformatics technologies were used to extract molecular scaffolds from the list of identified molecules before searching for related molecules in drug databases. In order to construct a biological network including viral species, molecules, scaffolds, drugs, and diseases supported by literature citations, the association between viruses and drugs that had been established was exploited. In addition, depending on how frequently they appear in the literature, we identified the top-ranking species and compounds. Furthermore, the molecular descriptors were calculated for the molecules obtained using Chemaxon and Molsoft, which can be further utilized for in-silico drug discovery like docking and dynamics.

Keywords: Virus, antiviral, biological network, literature mining.

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