

# MIT School of Bioengineering Sciences & Research

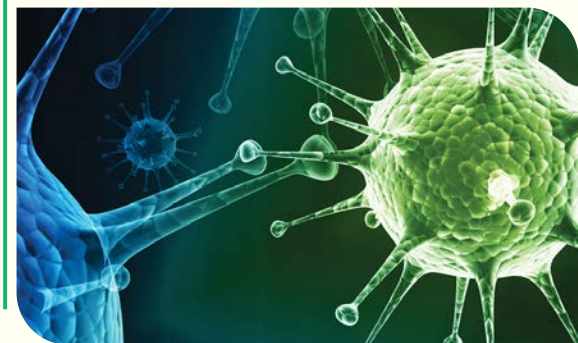
(A constituent unit of MIT ADT University, Pune India)

## 4<sup>th</sup> INTERNATIONAL CONFERENCE ON RECENT TRENDS IN BIOENGINEERING

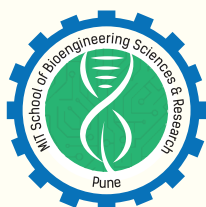
(ICRTB 2021)

February 12-13, 2021

## ABSTRACTS



The event will be held on virtual platform



MIT School of  
**Bioengineering Sciences  
& Research**

Breathe Life into Engineering Career!



**MIT-ADT  
UNIVERSITY**  
PUNE, INDIA

A Leap Towards The World Class Education

## About ICRTB 2021

ICRTB 2021 is the largest technical event in Bioengineering in India to foster interdisciplinary exchange and learning. Its goal is to bring together engineers, medical experts, researchers and practising clinicians, individuals working in academia, industry and government agencies.

## Conference theme areas

- Nanobiotechnology
- Synthetic Biology
- Tissue Engineering
- Environmental Biotechnology
- Wearables & Diagnostics
- Assistive Devices
- Nanoinformatics
- Immunoinformatics
- Drug Design
- AI and Big Data in Biology
- Biomedical Robotics
- Medical Image Processing

4<sup>th</sup> International Conference on  
**Recent Trends in Bioengineering**  
**(ICRTB-2021)**

**Editors**

**Prof. Vinayak Ghaisas**

**Dr. Renu Vyas**



**MIT School of Bioengineering Sciences &  
Research**

MIT, Art, Design and Technology University, Pune-412201,  
India



# *Messages*





**Hon. Prof. Dr. Vishwanath Karad**

*I am very happy to learn that the MIT School of Bioengineering Sciences & Research is organizing its annual flagship event- the 4<sup>th</sup> International Conference on Recent Trends in Bioengineering (ICRTB 2021). It is really amazing that despite the pandemic the enthusiasm of the staff and its leaders has been unhindered. ICRTB is one of my favourite events at MIT MAEER since it brings together professionals from different areas of expertise mainly doctors, scientists and engineers on a common platform for exchange of ideas and intellectual deliberations. My heart felt wishes to the organizers and warm welcome to the delegates.*

A handwritten signature in black ink, appearing to read 'Vishwanath D. Karad'.

**Prof. (Dr.) Vishwanath D. Karad**  
Founder, MIT Group of Institutions  
President, MIT- ADT University



***Hon. Dr. Suresh Ghaisas***

*With deep sense of satisfaction and contentment I wish to congratulate the organizers of the international conference for conducting this event regularly and also raising the standard every year. The list of speakers is amazing and being from medical fraternity looking forward to talks from professionals of medical schools.*

*Kudos to the convenors and blessings for rapid growth of the Bioengineering institute.*

A handwritten signature in purple ink, which appears to read 'S. Ghaisas', enclosed within a decorative, hand-drawn oval border.

***Dr. Suresh Ghaisas***  
*President and Trustee*  
*MIT MAEER*



**Dr. Mangesh Karad**

*Dear Delegates,*

*I would like to extend a warm welcome to all the delegates, industry guests, panellists and experts for this Annual Event.*

*With immense pride I announce the beginning of the 4th International Conference on Recent Trends in Bioengineering (ICRTB 2021) by MIT School of Bioengineering Sciences & Research.*

*I strongly believe in the resilience of human spirit and am sure the deliberations at the conference will be even more vibrant as healthcare is being increasingly brought into focus. My congratulations to the Bioengineering Institute for the interdisciplinary research and innovation culture nurtured at the institute that has brought several laurels to the university at national and international fora. Kudos to the convenors for organizing the event despite several constraints due to the prevailing health conditions globally.*

*Also on behalf of MIT ADT University I invite you to visit our beautiful campus whenever the situation is favourable.*

**Hon. Dr. Mangesh Karad**

*Executive President*

*MIT-ADT University*



**Prof. Vinayak Ghaisas**

*It gives me great pleasure to host our 4<sup>th</sup> International Conference in Recent Trends In Bioengineering. This conference is a great platform that brings doctors, clinicians, engineers, scientists as well as multiple industry experts on one platform to discuss, exchange and improve our collective knowledge in Bioengineering. Such great exchange of thoughts will result in great ideas, which we all would want to become products and benefit humanity.*

*Covid pandemic has not stopped our indomitable spirit to host this conference. We will be hosting this conference virtually with even greater participation of delegates and speakers around the world.*

*I wish extend a warm welcome to all our delegates, speakers & dignitaries.*

**Prof. Vinayak Ghaisas**

*Founder Director*

*MIT School of Bioengineering Sciences & Research*

*Managing Trustee, MAEER Pune*



**Dr. Renu Vyas**

*Warm welcome to all delegates, invited guests and speakers to the 4<sup>th</sup> International Conference on Recent trends in Bioengineering (ICRTB 2021). Extremely grateful to all our faculties who encouraged me to go ahead with this event and thanks to technology for bringing us together once again despite the pandemic. The event is growing larger each year in terms of international outreach, quality of the research papers and profile of the speakers. Very grateful to the delegates for participating in large numbers and sending abstracts on time. This year one of the theme of the conference is Digital Health and we have wonderful speakers from medical schools as well as industry who will delve into this topic and provide their insights.*

*ICRTB was initiated in 2017 to serve as a robust platform for cross pollination of ideas and a catalyst for translating research into products. It has served the purpose well and hope in coming years it will continue. Further another highlight of the present conference will be the launching of the OMIK Association of Bioengineering that will work throughout year for providing Bioengineering solutions to real world problems.*

*Once again thanks for joining us,*

**Dr. Renu Vyas**  
Head of the School  
MIT School of Bioengineering Sciences and Research  
Convenor ICRTB 2021



# ***Eminent Speakers***





***Aliasger K. Salem, Ph.D., FAAPS, FAIMBE***

*Bighley Chair of Pharmaceutical Sciences*

*Professor of Pharmaceutics, Chemical and Biochemical Engineering,  
Biomedical Engineering, Chemistry and Dentistry*

*Co-Leader, Experimental Therapeutics Program, Holden Comprehensive  
Cancer Center*

*Co-Director, Nanotoxicology Core, Environmental Health Sciences Research  
Center*

*Department of Pharmaceutical Sciences and Experimental Therapeutics,  
College of Pharmacy, University of Iowa*

*115 S. Grand Avenue, S228 PHAR*

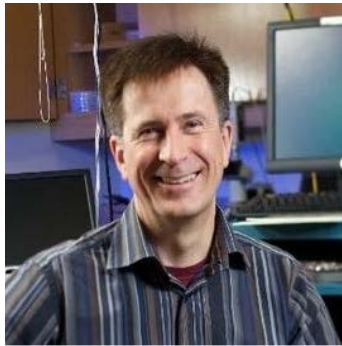
*Iowa City, IA 52242 | Phone: 319 335-8810 | FAX: 319 335-9349 |*

*aliasger-salem@uiowa.edu*

***Profile:***

Dr. Salem has extensive research leadership experience and specific and extensive peer-reviewed expertise in the development and testing of novel cancer therapies and cancer drug delivery formulations. Dr. Salem has served as Leader of the Experimental Therapeutics Program at the Holden Comprehensive Cancer Center for the last 9 years. Dr. Salem is a nationally prominent cancer therapeutics development and formulation expert as evidenced by his election to Fellow of the American Association of Pharmaceutical Scientists and his election as Fellow of the American Institute for Medical and Biomedical Engineering. In 2020, Dr. Salem was awarded the Hancher-Finkbine Medallion and the Leadership in Research Award by the University of Iowa for life-time achievements in research over his career to date. Dr. Salem has experience as the PI/PD of a wide range of private foundation and federal grants as well as his tenure as the Bighley Chair and Professor of Pharmaceutical Sciences. Dr. Salem

currently mentors one T32 surgical resident, one research scientist, 3 postdoctoral fellows and 19 PhD graduate students. He has previously graduated 24 PhD students under his primary mentorship with each former student going onto academic, government and industry positions.



***Dr. Karl F. Böhringer***

*University of Washington*

*Institute for Nano-engineered Systems (NanoES)*

*Seattle, WA 98195*

*Tel. 206 221-5177, fax 206 543-3842*

*karlb@uw.edu*

***Profile:***

Karl F. Böhringer received his Dipl.-Inform. degree from the University of Karlsruhe, Germany in 1990 and his M.S. / Ph.D. degrees in computer science from Cornell University, Ithaca, NY in 1993 / 1997. He was a Visiting Scholar at Stanford University in 1994-95 and a Postdoctoral Researcher at the University of California, Berkeley from 1996 to 1998. He joined the University of Washington in Seattle, WA in 1998, where he is currently Professor of Electrical & Computer Engineering and Bioengineering, Director of the Nano-engineered Systems Institute, and Site Director for the University of Washington / Oregon State University node in the NSF National Nanotechnology Infrastructure Network. He held visiting faculty positions at the Universities of Tohoku, Tokyo, Kyoto (Japan), São Paulo (Brazil) and École Polytechnique Fédérale de Lausanne (Switzerland).

Karl F. Böhringer is a fellow of IEEE. His awards include the John M. Fluke Distinguished Chair of Engineering at the University of Washington in 2010, an Invitational Fellowship for Research in Japan by the Japan Society for the Promotion of Science (JSPS) in 2004, an IEEE Robotics & Automation Society Academic Early Career Award in 2004, an NSF CAREER Award in 1999, and an NSF Postdoctoral Associateship in 1997. His work was listed among the “Top 100 Science Stories of 2002” in Discover magazine. He has served as editor for

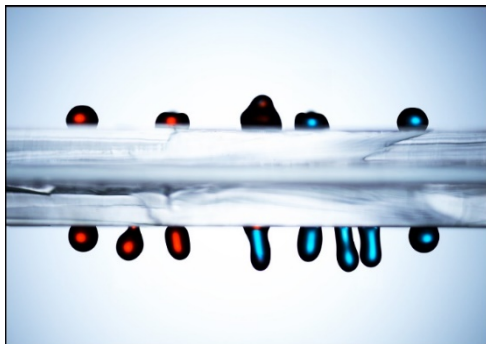
ASME/IEEE Journal of Microelectromechanical Systems, IEEE Transactions on Automation Science and Engineering, Frontiers in Mechanical Engineering and Microsystems & Nanoengineering. He has served, among others, on the technical program committees for the IEEE International Conference on Microelectromechanical Systems (MEMS) and the International Conference Solid-State Sensors, Actuators and Microsystems (Transducers) conferences, and he was general co-chair of IEEE MEMS in 2011.

### ***Talk synopsis***

#### **Moving Drops on Micro-structured Surfaces**

##### **Abstract**

The dynamic interaction between liquid drops and a solid surface is greatly influenced by its microscopic structure, including its topography and material composition. While phenomena such as capillarity and hydrophobicity have been studied for many years, recent research has produced remarkable new insights in this field. Here, we review the physical principles that produce movement of drops, develop models for their behavior, discuss the design and fabrication of micro-structured surfaces, and demonstrate several applications including a microfluidic platform for parallel processing of liquid samples and self-cleaning surfaces.



*Sessile and pendent drops moving on a surface  
with anisotropic microtexture*



***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](mailto: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, the internalisation routes taken by synthetic nanoparticles on exposure to cells, and how cells respond to nanomaterials and nanosurfaces. His lab also develops novel 3D cell models allowing the quantitative study of cell behaviour at multiple scales, with applications in drug delivery. He has authored over 100 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](http://www.ucd.ie/hcs)). He is currently the Head of Subject for the discipline of Cell & Molecular Biology in UCD and the Vice Principal (International) in the UCD College of Science.



***Dr. Anurag Agrawal***  
*Director, at CSIR, IGIB India*

***Profile:***

Dr Anurag Agrawal is Director of the CSIR Institute of Genomics and Integrative Biology. After completing graduate medical education at the All India Institute of Medical Sciences, Delhi (1994), he further trained in Internal Medicine, Pulmonary Disease and Critical Care at Baylor College of Medicine, Houston, USA (2003), followed by a PhD in Physiology from Delhi University. His primary research is in respiratory biology and broader interests are in smart deployment of emerging technologies towards healthcare, where he serves on national thinktanks, co-chairs the Lancet and Financial Times commission on Governing Health Futures, and serves on related expert groups at the World Health Organisation and Global Partnership for Artificial Intelligence. He received the Shanti Swaroop Bhatnagar Prize, the highest govt scientific award of India, in 2014, and is an elected fellow of the Indian National Science Academy and the Indian Academy of Sciences.



**Mr. Dinanath Kholkar**

*VP and Global Head of Analytics & Insights at TCS  
India*

***Profile:***

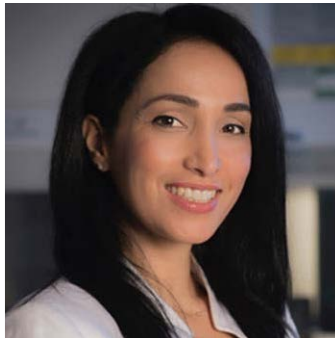
Dinanath Kholkar is Vice President Global Head, Analytics Insights at Tata Consultancy Services. In this role, Dina guides some of the world's best companies in their journeys to unlock the potential of their data through the power of analytics and artificial intelligence to uncover new business opportunities, drive business growth and increase revenue streams.

Dina has been recognized as one of the top 100 influential global data leaders and data visionaries. He advocates 'data centrality' as a strategic lever for business growth and transformation and believes that the need of the hour is 'of data analytics. His thought leadership in addition to his team's expertise and collaborative working with customer organizations is empowering them to realize the power of their data in real time decision making and ensuring success in their Business 4.0™ transformation journeys.

With over thirty years of industry experience, Dina has held diverse leadership roles across the organization and amplified business value to customer organizations covering all major industries. He was responsible for building TCS' data warehousing and data mining expertise and laying the foundation for the organization's Business Intelligence practice. Dina has also led TCS' Business Process Services (BPS) & Business Analytics units and served as the CEO Managing Director of TCS eServe.

Dina holds a Bachelor's Degree in Electrical Engineering. He has been providing industry leadership to the IEEE Pune section for over 15 years and was the Chairman for the Section between 2018-19

Dina is a member of the Board of Governors of his alma mater Veermata Jeejabai Technological Institute Mumbai and actively involved in the institute's alumni association. He is a Review Committee Member, Indian Statistical Institute, Kolkata and on the Advisory Committee of Pune Knowledge Cluster. He provides leadership, guidance and strategic direction in the fields of education, sustainability agriculture, and 'data for good' through his volunteering work at IEEE Pune Section, Pune International Center and Tata Group.



**Dr. Natalie Artzi**

*Assistant Professor at Brigham and Women's Hospital, Harvard medical School  
Principal Research Scientist at MIT, and a Founder of Biodevek.*

**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 using Materials: New Opportunities for Precision Delivery**

The generic use of an 'inert' vehicle that delivers a cargo to treat a range of cancer types and disease states obeys the 'one material fits all' rule. However, in

the absence of mechanistic understanding of the underlying biology and immunology, this approach leads to suboptimal and unpredictable clinical outcomes. The key factors constructing the tumor milieu should guide the design of disease-responsive materials that can be administered locally to release embedded drugs over time. Given the growing availability of polymeric scaffolds and nano-materials for cancer therapy, a biologically-informed material that responds to each patient's needs and reacts in a graded manner based on disease cues, would pave the way for precision materials for cancer therapy. Our main focus is to rationally design personalized materials based on specific disease-traits—biological signatures— that in turn facilitate efficacious and selective cargo delivery to the target cancer cells, while sparing normal cells. We leverage combination therapy—drug delivery, gene therapy and thermal ablation— and a variety of administration routes—local and systemic administration— to enhance treatment efficacy, while minimizing side effects. Our recent publications demonstrate that our approach results in tumor remission and with the prevention of tumor recurrence in mice.



**Prof. Pawan K Dhar**

*Dean, School of Biotechnology and Chair, Intellectual Property Cell,  
Jawaharlal Nehru University, New Delhi.*

**Profile:**

Prof. Pawan K Dhar is the Dean & Head, Synthetic Biology group, School of Biotechnology, JNU. Prior to this he held faculty positions at Shiv Nadar University, Symbiosis University (Pune), Kerala University, RIKEN Institute (Japan), Bioinformatics Institute (Singapore), Keio University (Japan) and Kyoto University (Japan) and Manipal University (Karnataka). Prof. Dhar received PhD in 1993 from BHU (Varanasi) for his work on Human Genetics. His work on making novel genes from intergenic DNA sequences has led to development of a novel drug discovery platform. This led to spinning of Foresight Biotech Pvt. Ltd, currently incubated at JNU, New Delhi. Prof. Dhar serves on the board of reviewers for European Science Foundation, DBT and MHRD.

**Talk synopsis**

**Synthetic Biology: concepts to applications**

For the last two decades, the scientific community has explored the possibility of applying engineering concepts in biology. This has led to rational design and construction of biological components, including parts, devices and circuits. In the first part of my talk, I shall outline the foundational concepts that led to a new field called synthetic biology. From the functional standpoint, broadly three kinds of DNA sequences exist: protein coding, RNA coding DNA and NOT coding. We asked a simple question: How did nature decide to allocate protein coding and RNA coding jobs to a specific set of sequences? Given the availability of enormous information in the neighborhood, did she sample all possibilities, retaining good results (protein and RNA encoding genes), retiring the not-so-relevant results (pseudogenes), leaving some genome sequences untouched (non-expressing genome). In the second part of my talk, I shall describe our work on not-coding DNA and provide proof of the concept.



***Dr. Shailaja Saxena***

*Head, Molecular Medicine and Regenerative Medicine, Reliance Life Sciences,  
India*

***Profile:***

A gold medallist MMBS, let go of her practicing medicine to be part of the corporate world. She doesn't fear taking chances and doesn't regret a bit. She heads Molecular medicine and Regenerative Medicine verticals at Reliance life sciences. Reliance Life Sciences was her first job soon after she returned from London after completing her Masters. She is associated with Reliance for more than 18 years now and she had seen RLS grow.

She did her MBBS from MGM Medical College, Indore with a gold medal and distinction. "Being the daughter of a renowned IVF specialist, everyone thought I would take after my father. In the final year though, I got to know of a particular course offered by a university in London that interested me. I discussed it with my father and to my pleasant surprise, he asked me to take a chance. All my friends and relatives tried to convince me to practice medicine, but research was my true calling. That is when I pursued my MSc in Prenatal Genetics and Fetal Medicine from University College London", says Shailaja.

Years later, she pursued a PhD from Mumbai University as part of continued educational program and completed it while on the job.



***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.



***Dr. Shailesh Puntambekar***

*Medical Director, Galaxy Care Hospital, India*

***Profile:***

Dr. Shailesh Puntambekar is a Medical Director at Galaxy Care Hospital, India. He conducted India's First Successful Laparoscopic Assisted Uterine Transplant. He has patented the technique of radical hysterectomy "Pune Technique" of Laparoscopic Radical Hysterectomy. Dr. Puntambekar is the only Indian to be the Board Member in AAGL (American Association of Gynae Laparoscopists), Faculty and member of AAGL Oncology Committee. He is operating Faculty at IRCAD and various other International organization and their conferences.

Dr. Puntambekar is known for performing the most difficult Laparoscopic/Endoscopic surgeries. He is a pioneer of Laparoscopic anterior/posterior exenteration for colorectal/uterine malignancies. Dr. Shailesh Puntambekar has been awarded the prestigious "Foundation Signature Award" from AAGL recognized all over the world as "The Golden Telescope Award". He has received the same award from AAGL four times in the past for his excellent work and this is the 5th Award.

Dr. Shailesh Puntambekar has been selected as International Secretary Treasurer for AAGL. He will be the first person to hold this prestigious position and will work closely with the AAGL board to promote and teach laparoscopy internationally.



**Dr. Justin Dauwels**

*Associate Professor,*

*Circuits and Systems, Department of Microelectronics TU Delft Mekelweg 5,  
2628 CD Delft*

*J.H.G.Dauwels@tudelft.nl*

**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 HenriBenedictus Fellow of the King Baudouin Foundation (2008), and a JSPS invited fellow (2010, 2011). He is active in the IEEE community as C hairman of the CIS Chapter in Singapore, AE of Trans on IEEE Signal Processing, and organizer of conferences and special sessions. 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***

Many tasks in medicine still involve substantial manual work. In many cases there is strong potential for intelligent automation by Artificial Intelligence (AI), 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 AI in the domain of neurology. We are developing a low cost validated system to automatically interpret EEG via remote access. Diagnosis and management of neurological disorders rely on visual review of EEG data by specialized physicians. As the duration of EEG recordings ranges from 30 minutes to several weeks, the visual review is time consuming, and accounts for approximately 80% of total cost associated with EEG reading. Our system has the potential to reduce expenses associated with EEG testing and allows physicians to devote more quality time to their patients. One of the applications that we have explored so far is diagnosis of epilepsy of EEG. In this talk, we will show numerical results on large EEG datasets of epilepsy patients and healthy control subjects for multiple centers.



***Dr. Hemant K. Gautam***

*Institute of Genomics and Integrative Biology  
Mall Road, University Campus Delhi-110007 India  
hemant@igib.res.in*

***Profile:***

Dr. Hemant K. Gautam obtained his Masters and Ph.D. degree in microbiology from the (I.A.R.I), New Delhi, India . He did post doctorate from France and Israel. He is currently working as a Senior Principal Scientist and Professor at Institute of Genomics and Integrative Biology, New-Delhi. He is associated with a number of Universities and members of various scientific and academic organizations. He is a recipient of SARC award, Bharat Excellence award, Biotechnology award, Israel Govt. Fellowship, UNESCO fellow & Intl. Project Reviewer RBUCE-UP, UniverSud, Paris, He has published more than 75 research papers, two books and over 500 new sequences have been submitted to NCBI database. He has visited several countries, including France, Israel, Australia, Bulgaria, China, Thailand, Germany, USA, Singapore, Vietnam, Malaysia and Ukraine. He has a distinguish background in the field of microbial biotechnology, microbiome, natural products, enzyme immobilizations, biosensors and microbial genomics. Currently he is working in the area of microbial biotechnology, antimicrobial resistance in skin & acne diseases.



**Mr. Nikhil Malhotra**  
*Global head of innovation,  
Creator of Maker's Lab  
Tech Mahindra, India*

***Profile:***

Mr. Nikhil is the Chief Innovation Officer and creator of Maker's Lab, a unique Thin-q-bator space within Tech Mahindra with 20+ years of experience. Nikhil has been a researcher all his life and is now leading the growth of AI, machine learning, robotics and quantum research within Tech Mahindra. Nikhil's area of personal research has been how quantum computing and neuroscience has inspired the growth of AI and how the two fields can merge in the future. Nikhil has also designed an indigenous robot in his lab, as a personal assistant. The current bets he has undertaken is how quantum can give us better cancer drugs, GANs and their application for languages and SPACE tech.

One of his vision is to enable machines to talk in local Indian dialect. There are 1645 dialects in India and 26 mother tongues and 80% of Indian population does not speak English. Nikhil is researching on Sanskrit and how this ancient Indian language could sow the seed for the next computer revolution.

He holds a master's degree in computing with specialization in distributed computing from Royal Melbourne Institute of Technology, Melbourne.



***Dr. Himanshu Gadgil***  
*Director and CSO*  
*Enzene Biosciences Ltd., India*

***Profile:***

Dr. Himanshu Gadgil is the Chief Scientific Officer and is responsible for all operations at Enzene. He holds a PhD in Biochemistry, and has a proven track record of managing multi-layered organizations toward successful global product launches of Biosimilars and development of Block-buster novel Biologics. He is a passionate innovator with over 50 publications/patents in field of Biologics drug development. Dr. Gadgil has a PhD in Protein Purification, Biochemistry from The University of Tennessee Health Science Center, Memphis, USA and post doc from UT Medical Centre. Prior to joining Enzene, Dr. Himanshu Gadgil was associated with Intas Biopharmaceuticals, Amgen and Waters Corporation.



***Dr. Dhanasekaran Shanmugam***

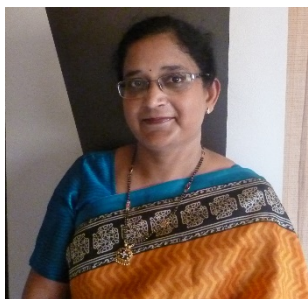
*Sr. Pr. Scientist, Biochemical Science Division, CSIR-National Chemical Laboratory, India*

***Profile:***

Dr. Dhanasekaran Shanmugam is a senior Principal Scientist at Biochemical Science Division, CSIR-National Chemical Laboratory, Pune, India. Dr. Dhanasekaran received his PhD from Indian Institute of Science, Bangalore, India in 2004. After that he worked as a Post Doctoral Research Fellow with Prof. David S. Roos, University of Pennsylvania, Philadelphia, USA from 2004-2011.

Research work in Dr. Dhanasekaran's laboratory is focused on studying cellular metabolism in apicomplexan parasites such as *P. falciparum* and *T. gondii*. Their interest is to understand various aspects of metabolic adaptation evolved by these parasites to sustain a parasitic life style and exploit unique and essential aspects of these metabolic features for identifying novel chemical inhibitors as leads for drug discovery. The approaches employed by his group include a combination of genomic, biochemical, genetic and metabolomic techniques.

The broad research areas includes Human Diseases, Enzymology and Microbiology, Molecular biology, Structure Biology, Chemical Biology, Proteomics and Metabolomics and Theory and Computational Science.



***Dr. Beena Rai***  
*Principal Scientist at TCS*

***Profile:***

A Ph. D from India's premier research institution – **National Chemical Laboratory, Pune**, Beena joined Tata Consultancy Services (TCS) two and half decades ago. Currently she leads Physical Sciences Research Area in TCS Research. Her pioneering research in Computational Material Engineering, especially leveraging physics-based models and data analytics tools and techniques in the design, development & deployment of materials and chemicals has led to the creation of **top-notch research papers (150+) and 80+ patent applications**. Her research has not only been instrumental in getting significant mindshare of TCS Customers but also resulted in significant dollar values.

She is a recipient of prestigious **Chevening Scholarship at Said Business School, University of Oxford, UK**. She has received several recognition and awards, to name a few: **TCS Distinguished Scientist Award, Distinguished Alumnus of National Chemical Laboratory Pune, Indian Institute of Minerals (IIME) Mineral Beneficiation Award, Vasvik Research Award** in Materials and Metallurgical Sciences and Technology for Women Scientist, **Materials Research Society of India Medal, SAIL Gold Medal, Maha-Intrapreneur Award** instituted by Praj Industries and Symbiosis International Institute of Business Pune, India and **WILL Best Mentee Award** given by WILL-Women in Leadership Forum, India.



## **Governing Body**

|                                   |                                                        |
|-----------------------------------|--------------------------------------------------------|
| <b>Dr. Vishwanath D. Karad</b>    | President                                              |
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# 4<sup>TH</sup> INTERNATIONAL CONFERENCE ON RECENT TRENDS IN BIOENGINEERING (ICRTB-2021)

(FEB 12 – FEB 13, 2021)

## Online Platform Detailed Schedule

### Day 01: 12<sup>th</sup> February Friday 2021

|                            |                                                                                                                                                        |
|----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|
| 8.30 am to 9.30 am         | Spot registrations, logins by guests, speakers and delegates                                                                                           |
| <b>9.30 am to 10.30 am</b> | <b>Inaugural program presided by Hon Vishwanath Karad sir, Founder MIT Group of Institutes and President MIT-ADT University</b>                        |
| 9.30 am to 9.35 am         | Welcome of audience by the anchors, World Peace prayer and digital lamp lighting                                                                       |
| 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 Bioengineering and Managing Trustee MAEER Pune                                            |
| 9.50 am to 10.00 am        | Brief remarks by Guest of Honour, Dr Virendra Ghaisas, Executive Director MIMER Medical College                                                        |
| 10.00 am to 10.20 am       | Inaugural talk on Bioengineering Trends by Chief Guest, Dr Aliasger, FAAPS, FAIMBE, Bighley Chair of Pharmaceutical Sciences, University of Iowa, USA. |
| 10.20 am to 10.25 am       | Speech by Prof Mangesh Karad, Executive President, MIT ADT University                                                                                  |
| 10.25 am to 10.35 am       | Motivational Talk by Hon. Vishwanath Karad sir Founder MIT group of institutes.                                                                        |

|                         |                                                                                                                                                                                   |
|-------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10.35 am to 10.40 am    | Release of abstract book and CD and inauguration of OMIK Association of Bioengineering by Director                                                                                |
| 10.40 am to 10.45 am    | Vote of Thanks by Dr. Vyas, Head of School, MITBIO                                                                                                                                |
| 10.45 am to 11.00 am    | Tea break and inauguration of e poster session by Dr Ajay Vishwakarma CEO, Cell BioEngines USA                                                                                    |
| <b>11.00 am to 1 pm</b> | <b>Keynote addresses (Session Chair: Prof. Vyas)</b>                                                                                                                              |
| 11.00 am to 11.30 am    | Professor Jeremy Simpson, UCD Ireland, on Engineering the Cell                                                                                                                    |
| 11.30 am to 12 .00 pm   | Dr. Karl Bohringer, University of Washington USA, on Microfluidics and Sensors                                                                                                    |
| 12.00 pm to 12.30 pm    | Dr. Dinanath Kholkar VP TCS India, Global Head Analytics and Insights, on Digital Health                                                                                          |
| 12.30 pm to 1 pm        | Virtual tour of Bioengineering labs in MITBIO Building 1 and 2                                                                                                                    |
| 1 pm to 2 pm            | Lunch Break , e poster session and Industry Expo                                                                                                                                  |
| <b>2 pm to 4 pm</b>     | <b>Plenary Session I</b>                                                                                                                                                          |
| 2 pm to 2.20 pm         | Dr. Justin Dauwels, Tu Delft Netherlands                                                                                                                                          |
| 2.20 pm to 2.40 pm      | Dr Dhanasekharan, Senior Principal Scientist, CSIR-National Chemical Laboratory, Pune                                                                                             |
| 2.40 pm to 3.00 pm      | Dr Shailaja Saxena, Head Molecular Biology, Reliance Life Sciences, Mumbai                                                                                                        |
| 3.00 pm to 3.20 pm      | Dr Natalie Artzi, Harvard Medical School USA                                                                                                                                      |
| <b>3.20 pm to 4 pm</b>  | <b>Tea break and e posters evaluation</b>                                                                                                                                         |
| 4.00 pm to 4.20 pm      | <b>Panel Discussion</b> on <i>Digital Health Care</i> (Panelists: Dr Beena Rai, TCS, Prof. Vinayak Ghaisas MITBIO, Dr Justin Dauwels, TuDelft, Dr Nikhil Malhotra, Tech Mahindra) |
| 4.20 pm to 6.20 pm      | Oral presentations by delegates (parallel sessions)                                                                                                                               |
| 6.30 pm                 | Day One Conclusion                                                                                                                                                                |

## Day 02: 13th February Saturday 2021

|                         |                                                                |
|-------------------------|----------------------------------------------------------------|
| 8.30 am to 9.30 am      | Industry Expo /Poster session                                  |
| <b>9.30 am to 11 am</b> | <b>Key Note Addresses (Session Chair: Prof. Vyas)</b>          |
| 9.30 am to 10 am        | Dr Anurag Agarwal, Director, CSIR IGIB New Delhi               |
| 10 am to 10.30 am       | Dr Shailesh Puntambekar, Director Galaxy Care Hospitals Pune   |
| 10.30 am to 11 am       | Dr Nikhil Malhotra, Global Innovation Head, Tech Mahindra Pune |
| 11.00 am to 11.10 am    | Tea Break, e poster session, industry expo                     |

|                        |                                                                                                                        |
|------------------------|------------------------------------------------------------------------------------------------------------------------|
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| 11.10 am to 11.30 am   | Dr Pawan Dhar Dean, Biotechnology JNU New Delhi                                                                        |
| 11.30 am to 11.50 am   | Dr. Nathan Johnson, Harvard Medical School MA USA                                                                      |
| 11.50 am to 12.10 pm   | Dr Himanshu Gadgil, Director Enzene Biosciences Pune                                                                   |
| 12.10 pm to 12.30 pm   | Dr Hemant Gautam, IGIB New Delhi                                                                                       |
| 12.30 pm to 1.30 pm    | Lunch and Industry Expo                                                                                                |
| 1.30 pm to 4.30 pm     | Oral presentations by delegates (parallel sessions)                                                                    |
| <b>4.30 to 5.30 pm</b> | Valedictory function, announcement of Prizes, feedback from delegates, concluding remarks by Director, National Anthem |
| 6 pm                   | Conclusion of program                                                                                                  |



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# ***Paper Presentation***



## **Identification and Screening of Novel Anti-Cancer Compounds for Aurora Kinase A from Chemical Database**

Ipsa A. Singh<sup>1</sup>, Kiran Bharat Lokhande<sup>1</sup> and K. Venkateswara Swamy<sup>1,2\*</sup>

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**Abstract:** Aurora kinase, a group of enzymes belongs to serine-threonine family and plays a critical role in cellular division. AURKA is overexpressed and distribute beyond the nucleus in cancer cells and involved in the tumor genesis through multiple mechanisms. So, AURKA is used as a drug target for cancer. Flavones are a class of flavonoids which are present in plants which shows anticancer activity. Hence, the study will be on molecular binding modes between the derivative compounds of flavone containing fluoro groups and the Aurora kinase A. Similar compounds of 2'fluoroflavones, 3882 compounds are retrieved from PubChem database. Then drug like filters viz. REOS and PAINS were applied to remove toxic compounds using Canvas software. In order to investigate the binding mechanism of filtered 2449 compounds with AURKA (PDB ID: 2J47), docking was done using Glide (Schrödinger) software. The lead compound among above compounds were selected on the merit of hydrogen bonding, salt bridge as well as pi-pi interactions, 4-(6-Fluoro-4-oxychromen-2yl) benzoic acid has been found one of the best molecule from docking studies. The binding mode of lead compound with AURKA reveals that the amino acid residues viz, Lys162, Ala213 and His280 are more important for binding and having best binding energy (-10.059 kcal/mol) was noted among the ligand dataset. The 10ns MD simulations of Aurora A and lead compounds confirms thermodynamic stability as compared to standard compound. These result enhances further in vitro and in vivo experimentation and can probably serve as an ideal molecule for cancer treatment..

**Keywords:** Aurora kinase A, fluoroflavones, chemoinformatics, glide docking, md simulation.

## **Triamcinolone as a potential inhibitor of SARS-CoV-2 main protease and cytokine storm via molecular docking, molecular dynamics simulation, and free energy calculation**

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**Abstract:** The emerging COVID-19 pandemic triggered by acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is an ongoing global public health concern. However, there is no available medication to date for treating the COVID-19 infection effectively, which underscores the science that needs to be tackled. In view of the readiness problem created by COVID-19, the potency of current medications may be enhanced by the drug repositioning approach. Mpro is a main protease of SARS-CoV-2 has been established as a potential drug target because of its direct role in viral replication and ability to infiltrate multiple host pathways. This research aims to classify new therapeutic drug candidates which may be repositioned for COVID-19 therapeutics. In our current research work, we have taken similar drug compounds of Dexamethasone and conducted virtual screening by using computer-aided drug design approach. We targeted the main protease of SARS-CoV-2 (Mpro) along with the key molecules involved in the 'Cytokine storm' among the COVID-19 patients, i.e., TNF- $\alpha$ , IL-6, and IL-1 $\beta$ . Further we did MD simulations and calculated molecular mechanics/Poisson-Boltzmann surface area (MM/PBSA) on the active site of the main protease of SARS-CoV-2 (Mpro) and TNF- $\alpha$ , IL-6, & IL-1 $\beta$  to explore the binding affinity and stability. Based on our study outcome, Triamcinolone emerged as the most promising inhibitor of the main protease of SARS-CoV-2 (Mpro) and the cytokine storm molecules, i.e., TNF- $\alpha$ , IL-6, and IL-1 $\beta$ . However, it's important to remember that Triamcinolone requires more study in the in vitro and in vivo sense. This research investigates the repositioning of COVID-19 drugs as a new therapeutic application.

**Keywords:** COVID-19; main protease Mpro; Triamcinolone; protease inhibitor; cytokine storm suppressor; molecular docking; MD simulation

### **3D-printed antimicrobial face protective device against COVID-19**

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**Abstract:** Novel Corona virus, a pandemic of respiratory disease spreading from person-to-person. This situation is currently highly alarming with a very serious public health risk which may leads to death. In the wake of spurt in multiple cases of coronavirus pandemic in the country, the Ministry of Home Affairs, Government of India on March 14, 2020 has decided to treat Covid-19 as a Notified Disaster. To help the country in fighting coronavirus through quick validated prototype/product development and deployment we made an attempt in terms of developing protective gears to avoid the spread of COVID-19 transmission from infected person to non-infected. We arrived to a solution to fabricate a 3D printed object to avoid further passing on COVID-19 transmission from one person to others. Thereby, we designed, developed and prototyped a 3D printed antimicrobial face protective device using PACTIVE AN1™ (an innovative Copper-embedded antimicrobial including anti-viral property) with a high quality Poly-lactic acid (PLA) filaments which is used to make the 3D printed horizontally positioned head shield prototypes whereas, Fluorosilicone coated polyester film, having an excellent antimicrobial and anti-biofilm efficacy, was used to integrate with the 3D printed fabricated head shield object that act as a front-transparent, highly occlusive facial shield. The interesting features are: easy-to-design, rapid development of the prototypes, low cost, easy to wear, antimicrobial face shield, transparent, excellent chemical stability, non-fragile and easy to clean with the existing sanitizers or any alcoholic disinfectant.

**Keywords:** 3D printing, antimicrobial, headgear, face-shield, COVID-19.

## Evaluation of the antibiofilm efficacy of a newly designed compound against surface wound associated infections: an in-silico and statistical approach

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**Abstract:** Biofilm is consortia of sessile group of microbial species that adhere to biotic and abiotic surface with the help of extracellular polymeric substances (EPS) and glycocalyx. Wound is a lesion on the epidermal surface, that exposes the underlying tissues to the external environment and thus forms a region of proliferation for several species of *Staphylococcus* and *Streptococcus*. The in-silico studies performed on biofilm forming bacterial proteins revealed the role of various known bioactive compounds (viz. sclerin, nimbin, 5-Hydroxymethylfurfuryl and curcumin) in comparison to a newly designed compound (L) in the eradication of biofilm formation by some of the most popular Gram-positive surface wound infection causing strains (such as *Staphylococcus aureus*, *Staphylococcus epidermidis* and *Streptococcus mutans*). The selected ligands were thoroughly observed for its molecular electrostatic property and molecular docking was done to predict the 2D protein-ligand interactions. The optimization of interaction for the compound L was initially performed using response surface methodology (RSM) and artificial neural network (ANN). It was observed that the R<sup>2</sup> value for RSM was 0.75 and ANN was 0.9, which indicates it significant molecular interaction with the biofilm forming protein. It was further observed that the newly designed compound shared all drug-like properties and showed maximum interaction with the biofilm forming protein using Schrodinger (-33.75Kcal/mole with *S. epidermidis*, -36.064 Kcal/mole with *S. mutans* and -44.272 Kcal/mole with *S. aureus*). Thus,

this study provides a new dimension of antibiofilm compound (drug) which possess maximum potency of eradicating biofilm formed by the wound associated pathogenic biofilm causing virulent organisms.

**Keywords:** Surface wound biofilm, bioactive compound, docking interaction, RSM, ANN.

### **Removal of Zn<sup>2+</sup> ions from contaminated water using Cucumber Peels**

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**Abstract:** In the present study, Physico-chemical characterization and the adsorption behaviour of cucumber peels in the form of dried powder with regard to zinc (Zn<sup>2+</sup>) ions were studied in order to evaluate its importance to the purification of metal-contaminated water. The SEM micrograph shows the presence of irregular grooves and porous structures on the surface of the CPP. The FTIR study confirmed the presence of O-H & H-bonded OH on the surface, C=O amide and C-O-C phenol and cellulose. These functional groups along with porous surface aided in the removal of Zn<sup>2+</sup> ions. The batch approach was used and effect of pH (1-11), adsorbent dose (0.1-1 g), initial zinc ions concentration (10-100 mg/L) and contact time (0-300 minutes) were assessed on the adsorption of Zn<sup>2+</sup> ions by the cucumber peel powder (CPP). The optimum pH was 5, adsorbent dose was 0.1 g, adsorbate concentration was 100 mg/L and time of contact was 300 minutes for Zn<sup>2+</sup> ions removal. Langmuir isotherm ( $R^2 = 0.99$ ) and Pseudo second-order kinetics ( $R^2 = 0.99$ ) were fitted better and suggest monolayer adsorption with chemisorption mechanisms for Zn<sup>2+</sup> ions adsorption. Results have shown that CPP has the ability to remove zinc ions from contaminated water.

**Keywords:** Adsorption, cucumber peel, isotherm, kinetic, optimization, zinc.

## **Development of Nanoparticles by using *Erythrina variegata* against Breast Cancer treatment**

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**Abstract:** *Erythrina variegata* is also known as “Indian coral tree” and the leaves has anti-bilious, febrifuge, anti-helminthic, antiepileptic and anti-asthmatic properties hence used in ancient as well as traditional medicine in India, China and Southeast Asia. Silver nanoparticles (Ag NPs) importance and utility has been enhanced biomedical applications because of their large antimicrobial spectrum. Green synthesis of silver nanoparticles has uniqueness such as rapid, nontoxic and eco-friendly. It is a simple one-step alternative method over the other conventional physical/chemical techniques. Green synthesis of leaf extract of *E. Variegata* AgNP's confirmed successfully served as a reductants and capping agents, analysed by UV-Vis, FTIR, SEM-EDS, XRD and Zeta potential. An absorbance peak was observed at 350 – 420 nm range in UV Visible spectrophotometer. The size dimensions of Ag NPs with SEM were within the range of 59.5 to 99.2 nm. The AgNPs were analyzed as well as confirmed with Diffraction (XRD) and FTIR as naturally nanocrystalline as a face-centered cubic form (fcc) with flavonoids and terpenoids. Zeta potential analysis indicated the presence of more negative charge on the nanoparticles. Biological characterization of AgNP's shows the presence of terpenoids and saponins evaluated by phytochemical screening and these are responsible for 81% antioxidant activity at 25µg/ml. It was noted that antibacterial activity was similar to streptomycin as against gram +ve and gram -ve bacteria. In addition to this AgNP's, shows cytotoxicity assays decrease in cell viability of cancerous cell line MCF-7 of breast cancer at 0.156µg per 100ml and *invitro* haemolytic activity at higher concentration.

**Keywords:** *Erythrina variegata*, Ag nanoparticles, Antimicrobial activity, Anticancer activity.

## **Anti-Cancer Therapeutic Effects of Green ZnO Nanoparticles on 2D and 3D Cancer Models**

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**Abstract:** The fabrication of green nanoparticles has opened several novel avenues in biomedical science field like drug delivery, biosensor development, and tissue engineering. In the present study, we synthesized zinc nanoparticles (ZnO NPs) using the leaf aqueous extract of *Annona muricata* (*Am*) and characterized them using UV/Visible spectroscopy, FTIR spectroscopy, powder XRD, TEM, SAED, DLS and zeta potential measurement. The synthesized *Am*-ZnO NPs showed its optical absorbance at 355 nm and observed as spherical NPs with an average hydrodynamic size of about  $\sim 417$  nm and a net negative surface charge of  $\sim -2.59$  mV. The obtained *Am*-ZnO NPs are biocompatible and hemocompatible nature. The cell viability study was carried out for *Am*-ZnO NPs along with doxorubicin (DOX) as a positive control on 2D tumor model of pancreatic cancer (MIA PaCa-2 cells). We observed the anti-cancer therapeutic effect of *Am*-ZnO NPs. To understand the cancer cell death mechanism, we carried out apoptosis study and we showed a depolarization of mitochondrial membrane potential which is an intrinsic signature of apoptosis induction. Thus, cancer cells underwent programmed cell death. These results further substantiated on 3D tumor model (Tumor spheroids) that mimic with the tumor microenvironment conditions. We observed the size reduction of lung tumor spheroids in both NPs and DOX treatment. Conclusively, our study indicated that *Am*-ZnO NPs have anti-tumor effects on both 2D and 3D cancer models.

**Keywords:** ZnO, Nanoparticles, Anti-cancer, Apoptosis, Leaves extract, *Annona muricata*.

## **Multi parameter adaptive neuro fuzzy inference system model for blood oxygen saturation level maintenance of ventilated patients**

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**Abstract:** Sustaining the blood oxygen level of patients in mechanical ventilators is a serious issue faced by physicians in clinical intensive care units. Even in developed nations, health care specialists are manually adjusting various mechanical ventilator parameters periodically for maintaining oxygen saturation. In epidemic conditions where the patient number increases violently, automation of ventilator reduces the risk and effort of health care professionals. Real time maintenance of blood oxygen saturation level in pandemic situations can only be made possible by the application of modern machine learning assisted artificial intelligent control mechanisms. A blended model using multiple adaptive neuro fuzzy inference system (ANFIS) is developed here to predict the inspired oxygen output along with the corresponding ventilator mode for maintaining the blood oxygen saturation level within desired limits considering real time patient data and ventilator settings. Multiple ANFIS output of inspired oxygen and mode prediction is compared with physicians' decisions and it is found that the developed system output shows a very low error of deviation of less than 5% from physicians' prediction. Also, this method improves the speed of rule development compared with the general fuzzy inference model.

**Keywords:** Blood oxygen saturation, inspired oxygen, mechanical ventilation, artificial intelligence, adaptive neuro fuzzy inference system.

### **Review on Status quo of COVID-19 treatments**

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**Abstract:** Complementary and Alternative medicines (CAM) or other natural products on boosting one's immunity against COVID-19 have potential to improve or supplement existing standard of care available to prevent or treat COVID-19. Pandemic has brought the world's focus on health back again. COVID-19 has shown its high virulence in an immune-compromised population whereas it is generally mild in otherwise healthy people. It is hence, important to enhance the body's natural defense system using a healthy diet, and an active lifestyle to maintaining optimum health. A lot of organized scientific studies on therapies for COVID-19, both locally and internationally, are being quickly produced. Therefore, credible evidence supported by appropriate research is essential to ensuring public health in dealing with the current COVID-19 pandemic and improving public awareness on the undue promotion of fake medicine. Oleander teas, essential oils, siliver products have been tried without success in USA. In India, a sizable number of people affected with n-Coronavirus infection have tried Ayurvedic Kadha, a recommended formulation with subjective health benefits. Curcumin, a polyphenolic compound extracted from spice, used commonly in India, can potentially enhance the antibody response even if it takes at low doses. Curcumin is used as Golden Milk (Haldi milk) in India as a popular immunity boosting remedy against COVID-19 infection. Similarly, Vitamin D has been suggested to be one of the CAM potentially useful in boosting immunity. Much in the same way, limited evidence suggests that steam inhalation, saline gargles, nasal irrigation, and yoga could be useful as well. Experts have also been suggesting taking a holistic approach to general health focusing on immunity focusing on prevention before cure. Current review focuses on the role of Natural products and approaches against COVID-19.

**Keywords:** Complementary and alternative system of medicine, Natural products, COVID, Corona virus.

**DNA profiling of nine STR loci in Ediga community of Urban and Rural areas of Tirupati and Chittoor regions of Andhra Pradesh, India.**

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**Abstract:** The key intention of this project is to create a population DNA database by studying allele frequencies of 9 STR loci with a review of heterozygosity in Ediga population of Andhra Pradesh, India and correlate them with the compatible data for nearby populations for Forensic purpose. In this study we have chosen 40 extraneous families from Ediga (Idiga) population belonging to urban and rural places of Tirupati and Chittoor regions of Andhra Pradesh, India. Later on, we have selected one person from each family with unique surname and collected their blood samples for DNA profiling. Genotyping and allele frequencies of collected samples have been analyzed through profiling of nine STR loci. Along with allele frequencies and heterozygosity other forensic genetic parameters like effective number of alleles- $A_E$ , power of discrimination-PD, probability exclusion- PE, polymorphism information content-PIC, typical paternity index -TPI, exact test with Arlequin analysis and Bonferroni corrections were accomplished. STR (short tandem repetitive sequence) analysis of amelogenin and 9 loci namely D3S1358, vWA, FGA, D8S1179, D21S11, D18S51, D5S818, D13S317 and D7S820 was done from the extracted DNA through ABI 310 Genetic analyzer using Amp FISTR profiler® Plus<sup>TM</sup> amplification Kit.

Average heterozygosity observed across 9 loci in Ediga population was 0.6527. Our data indicated the relevance of STR markers in both forensic DNA analysis, DNA data bank and population genetics through determination of more precise dispersion of allelic frequencies and other forensic parameters.

**Keywords:** DNA profiling, allele frequencies, STR loci, Ediga, Heterozygosity.

**Synthesis and characterization of L-asparaginase Bionanoconjugate (BNc): A comparative *in-vitro* biophysical study of immobilized fungal L-asparaginase as an antineoplastic agent**

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**Abstract:** This paper describes the production of L-asparaginase from *Aspergillus terreus* BV-C strain along with preparation and characterization of L-asparaginase conjugates with silver and silica nanoparticles (Bionanoconjugates or BNc). The suggested possibility of the increase in stability of drugs once immobilized was also explored. Post synthesis and characterization, the particle size of silver nanoparticles was found to be  $9.70 \pm 11.54$  nm whereas the silica nanoparticles were found to be 27.46 nm. The encapsulation of free enzyme onto the Np also showed a drastic improvement in release profile under various physiological conditions such as temperature, pH and peptidase enzyme. The comparative study on *in-vitro* cytotoxicity on neoplastic cell lines such as HL-60, HeLa, JURKAT, K-562, PC-3 and MCF - 7 using Sulfo-Rhodamine B assay revealed the enhanced cytotoxic effect of the bioactive agent once encapsulated in a Np. The decline in cell growth percentage up to 50% after the administration of the BNc formulations showcased their great potential as an anticancer drug formulation also suggesting that encapsulation of a bioactive agent can increase its biocompatibility as a therapeutic agent.

**Keywords:** L-asparaginase, silver nanoparticle, silica nanoparticle, cytotoxicity, bionanoconjugate

## **Identification of lncRNAs in oral cancer subtype: A transcriptomic analysis**

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**Abstract:** Over the years long non coding RNAs or lncRNAs have been found to be involved in numerous fundamental processes of gene regulation. For example: Chromatin modification, DNA methylation, etc. Long non-coding RNAs, are non-protein coding transcripts which are longer than 200 nucleotides. This characteristic distinguishes them from small regulatory RNAs such as microRNAs (miRNAs), short interfering RNAs (siRNAs) and other short RNAs. When the lncRNAs are found to be differentially expressed, they pose the possibility to play a significant role in carcinogenesis. Presently oral cancer is considered as one of the most prevalent cancers affecting the human population along with its numerous subtypes. LncRNAs suffer an alteration in their expression due to a variety of factors, along with their involvement as regulatory factors in complex networks. Therefore the need to study about the mechanism and functions of the lncRNAs involved in the cancer reaches significant priority. Identification of long non coding RNAs as well as lncRNAs which are speculated to play a role in the mechanism and formation of various forms of cancer. For identification and analysis of lncRNAs, comparison between the expression of lncRNAs in normal and affected tissues will confirm the involvement of lncRNAs in the disease or the lack thereof. Similarly the dysregulated lncRNAs, will help us understand their relevance in tumor growth and maintenance.

**Keywords:** Oral cancer, long non coding RNA, epigenetics.

**Discovery of Aurora Kinase-B Inhibitors as Antitumor Drugs by 3D-QSAR, Molecular Docking and Molecular Dynamic Simulation Studies**

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**Abstract:** The serine–threonine kinase gene Aurora–B kinase plays critical role in spindle assembly, chromosome alignment, mitotic check–point activation and cytokinesis. The over expression of Aurora–B causing errors in cell division and multinucleation in centrosome numbers leads to cancer. Three–dimensional Quantitative Structure Activity Relationship (3D–QSAR) by PHASE module of Schrödinger suite was carried out for known inhibitors to find valid pharmacophore hypothesis. The five features hypothesis AADRR with better parameters ( $R^2=0.971$ ,  $Q^2=0.907$ ) using partial least square (PLS) analysis has been selected for virtual screening. Molecular docking was applied to find the probable binding mode interactions of ligands with Aurora–B binding pocket. Lys 106, Ala 157, Glu 161, and Phe 219 were identified as crucial residues formed several interactions with the ligands which are essential for Aurora–B inhibition. After different level of screening, five compounds from National Cancer Institute (NCI) database were acknowledged as novel inhibitors of Aurora–B. The active site interactions and the conformational stability of the protein–ligand complex were examined by molecular dynamics simulations studies.

**Keywords:** Aurora–B kinase, cytokinesis, 3D QSAR, docking; molecular dynamics.

## **Molecular signaling in Thymic Epithelial Cells Development and Homeostasis during Aging**

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**Abstract:** T cells, an essential component of the immune system, generate protective adaptive immune responses against pathogenic organisms and cancer cells. T cells are produced in the thymus, which provides a unique microenvironment needed for T cell development. Thymus consists of thymic epithelial cells (TECs) in the outer cortex and inner medulla provide signals required for the survival and differentiation of immature T cells, referred to as thymocytes. Medullary TECs (mTECs) play a critical role in preventing autoimmunity because they have the ability to express peptides found in other organs throughout the body. Presentation of self-peptides to thymocytes causes deletion of cells that express high affinity self-reactive receptors. Numerous studies including us have established that a major signaling pathway mediated by NFκB family members is indispensable for mTEC development. In the current study, we use gain- and loss-of-function genetic approaches to demonstrate that another pathway, mediated by Stat3 signaling, plays an important role in mTEC development and homeostasis. We show that the Stat3-mediated signaling pathway also plays a key role in mTEC development and homeostasis. Expression of a constitutively active Stat3 transgene targeted to the mTEC compartment increases mTEC cellularity and bypasses the requirement for signals from positively selected thymocytes to drive medullary region formation. Conversely, conditional deletion of Stat3 disrupts medullary region architecture and reduces the number of mTECs. Stat3 signaling does not affect mTEC proliferation, but rather promotes survival of immature MHCII<sup>lo</sup>CD80<sup>lo</sup>mTEC precursors. In contrast to striking alterations in the mTEC compartment, neither enforced expression nor deletion of Stat3 affects cTEC cellularity or

organization. These results demonstrate that in addition to the NFkB pathway, Stat3-mediated signals play an essential role in regulating mTEC cellularity and medullary region homeostasis. We are working on the influence of NFkB and Stat3 signaling pathway in TEC development and homeostasis during thymus involution.

### **Anti-cancer activity of TiO<sub>2</sub> nanostructures**

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Cancer has a major impact on public health all over the globe. Cancer has been treating by radiotherapy and chemotherapy, but these therapies had numerous side effects. Hence, it is very essential to find human safe drugs for the treatment of cancer. Nanotherapy becomes a prominent strategy to treat the cancer. TiO<sub>2</sub> nanomaterials are known to be non-toxic, stable and cost effective with several applications in biomedical sciences. We made TiO<sub>2</sub> nanoparticles and studied their anti-cancer activity by *in vitro* and *in vivo* methods. Our *in vitro* results showed that TiO<sub>2</sub> inhibited proliferation. Furthermore, TiO<sub>2</sub> nanomaterials decreased the migration and also colony formation of cancer cells. More importantly, TiO<sub>2</sub> exhibited anti-angiogenic property in CAM assay. Additionally, TiO<sub>2</sub> nanomaterials up regulated tumor suppressor genes. It has been shown that titanium dioxide nanotubes (TNT) and Quercetin (Qu) are effective anti-cancer agents. However, conjugated TNT with quercetin (TNT-Qu) as a combinational treatment is not know yet. We showed the anticancer activity of TNT-Qu in B16F10 melanoma cells. TNT-Qu significantly inhibited proliferation, migration and induced apoptosis in melanoma cells. Also, quercetin and TNT-Qu decreased the reactive oxygen species and superoxide levels due to quercetin antioxidant property. TNT-Qu exhibited enhanced anticancer properties and TNT-Qu could be a potential therapeutic combinational molecule for skin cancer treatment.

### 3D Structure Modeling of Human Telomerase Reverse Transcriptase

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**Abstract :** Human telomerase activity has been observed in 90% of cancers, thus validating it as a significant therapeutic target. However, a scarce number of drug candidates have reached clinical trials. One of the reasons for this anomaly is the limited knowledge of telomerase complete protein/enzyme 3D structure, more importantly that of its catalytic subunit – the telomerase reverse transcriptase (hTERT). Computational modeling has vastly supported the structure based drug discovery projects in last decade. With a poor template homolog from the Protein Data Bank, in the present work we have modeled the whole length of 1132 amino-acid sequence of hTERT using I-TASSER (Iterative Threading ASSEmbly Refinement). 5 distinct 3D structures of hTERT protein were generated with a c-score range from -0.98 to -1.98. Model-1 with highest c-score of -0.98 was considered for further evaluation. The model-1 from I-TASSER exhibited a ProSA score of -7.89 and Ramchandran plot analysis reported with 64% most favored regions, 27.4% additionally allowed regions, 5% generously allowed regions and 3.6% disallowed regions. The energy minimization was carried out using YASARA force field minimization server and reported Initial Energy to be -554223 kJ/mol and Final Energy to be -687718.6 kJ/mol. Further, the current modeled structure would be studied under MD simulation to understand its dynamic behavior in an appropriate solvent system and conditions and can be subjected to *in silico* based molecular interaction studies for detail drug designing mechanism.

**Keywords:** hTERT, Structure, I-TASSER, ProSA, YASARA.

## **Detection of Trace Elements by Molecularly Imprinted Polymers in Forensic Science**

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**Abstract :** In the field of forensic science, the most challenging aspect is to detect and identify trace elements from complex mediums. These evidences may be drug, toxin, DNA, fire accelerants, explosives, GSR etc. Forensic science is a growing field which needs effective analytical techniques and molecularly imprinted polymers (MIPs) can prove to be of great significance towards the modern day research. This technique has various applications in different fields such as in food industry, environmental analysis, in making biosensors, drug delivery systems, sample pre-treatment, separation/extraction due to its high stability, specificity, long shelf-life, robustness and cost effective nature. In this review, we focused to draw attention upon different approaches of this technique like detection, extraction and instrumentation with consideration of the previous literature. We intended to outline the significance of MIPs in the field of forensic science, to meet the current needs of criminal investigation with efficiency. This technique is yet to be explored in forensic science.

**Keywords:** Molecularly imprinted polymers, Forensic science, Trace elements

## **Role of Antioxidants in Cryopreservation Techniques for Longer Life of Human Spermatozoa**

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**Abstract:** Sperm cryopreservation has revolutionized the field of assisted reproduction and is also known to cause cryodamage to structure and function of spermatozoa during freeze thaw process. Different cryopreservation protocols and techniques mainly focus on the post thaw recovery of functional and genetically healthy spermatozoa including sperm DNA integrity and chromatin structure alterations. This study compared different freezing Medias commercially available to check the DNA integrity of sperms post cryopreservation which suggested the significant decrease in motility, viability and normal morphology after cryopreservation indicating the adverse effect of cryoprotectant on spermatozoa. Sperm apoptosis occurs due to excess production of Hydrogen peroxide which induces lipid peroxidation and fragmentation of DNA .Very less data is available on pregnancy rate and live birth rates. Cochrane review concluded about the increased and improved pregnancy as well as live birth rates using antioxidants. In Antioxidants only Vitamin E and Zinc have been reported for live birth rates. Studies showed that human sperm damage induced by freezing-thawing process can be potentially reduced by Antioxidant supplementation to freezing media. Improving the semen quality prior to cryopreservation, addition of proper and optimal cryoprotectant and also proper thawing protocols can successfully reduce the risk of potential DNA damage. Hence optimizing the criteria for post thaw spermatozoa and sperm cryopreservation in terms of poor quality semen is very essential to preserve male infertility.

**Keywords:** Antioxidants, infertility, male, oxidants, quality, sperm.

**Identification of *Salmonella sp.* in different food matrix by RTPCR in rapid and cost effective manner**

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**Abstract:** Identification of *Salmonella sp.* is crucial to maximize food safety. In cases with relatively low concentration of pathogens the conventional techniques causes a problem with detection, this is where real time PCR is one step ahead than all other methods of pathogen detection. In this study, Real Time Polymerase Chain Reaction (RTPCR) technique based on Sybr Green dye for detection of *Salmonella sp.* was used. Species specific primers were designed and their specificity was determined through Bioinformatics tools. The validation was done in terms of Specificity (specific for *Salmonella sp.* as compared to *E. coli*, *S. aureus*, *Listeria sp.* and *L. pneumophila*), Sensitivity (Post- amplification melting curve, Limit of Detection, Standard curve were analysed to determine primer-dimer formation and PCR amplification efficiency rate) and lastly Reproducibility and Repeatability with different food matrices (Meat samples, Vegetables samples and Milk samples) spiked with different concentration of *Salmonella* strain using different RTPCR machines. The limit of detection was determined up to 10<sup>2</sup> CFU/ml for *Salmonella sp.* The developed in-house method was validated in terms of sensitivity, specificity, reproducibility and repeatability for *Salmonella sp.* identification, within 5-6 hrs, which is a cost-effective and rapid method that would be useful for hotel industries, rail and air caterings for safety of consumers.

**Keywords:** *Salmonella sp.*, real time PCR, specificity, sensitivity, repeatability, and reproducibility.

## **Improvement of a life saver thrombolytic protein drug by Strategic Pegylation**

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**Abstract:** Cardiovascular diseases (CVDs) have upsurged world-wide including India the number of deaths worldwide in the last two decades. Apart from costly surgical interventions, thrombolytic therapies play a crucial role in combating CVDs. However, there is a dire need of an agent which is affordable, long-lasting and having clot-specificity so as to minimise the risk of bleeding as a side effect. Among various proven thrombolytics, Streptokinase is one of the preferred thrombolytic agents in developing countries as compared to its costlier counterparts. It degrades the fibrin network efficiently besides also induces the systemic activation of plasmin which enhances the risk of haemorrhage. In addition, due to its bacterial origin, it is also associated with high antigenicity and relatively short half-life.

In the present study, we have engineered novel Streptokinase derivatives and PEGylated them to minimise these disadvantages. We designed, expressed and purified novel SK forms, and PEGylated these molecules carrying specific mutations and/or truncations to produce lead variants exhibiting specific clinically advantageous properties. In comparison with nSK, Pegylated variants showed fibrin specific action mode in contrast to the unmodified native molecule even though the engineered constructs displayed comparable activity as the native streptokinase. In addition, these derivatives had diminished immune-reactivity- two features of tremendous clinical advantage in thrombolytic therapy in both heart attacks and thrombotic strokes.

We believe that these new strategically-engineered variants might prove to be superior thrombolytic agents having improved efficacy owing to an extended *in vivo* half-life, low immune reactivity and fibrin clot specificity.

**Keywords:** Cardiovascular diseases (CVDs), Streptokinase (SK), PEGylated, half-life.

## **LIGNIN HYDROGEL: PROPERTIES AND APPLICATIONS**

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**Abstract:** Polymers are the potential materials having wide array of applications in industry and are user friendly. Biopolymers have attracted researchers recently due to their low cost, biodegradability, and ecofriendly behavior. In view of this, lignin is has tremendous ability to replace many synthetic material to reduce pollution and energy consumption. In lignocellulosic material 18% -25% is lignin. Lignin so far has been recognized as a recalcitrant material in biofuel industry and generally is burnt for energy purpose. Biopolymeric hydrogels have great applicability in environmental, biological, and biomedical fields. Hydrogels are polymer based networks that are known to absorb water or aqueous solvent about thousand times of their dry weight. Depending on t he application properties of hydrogel can be custom-made. Strategies are employed to change or modify hydrogel chemical structure. Lignin is made of three monomers namely p-coumaryl, coniferyl, and sinapyl alcohols. Lignin has abundance of functional groups that makes it suitable for desired modification for the construction of hydrogel. However, very less research has been done in this respect. Generally, lignin hydrogels are prepared from alkaline or kraft lignin using various modifiers that develop either physical crosslinking or chemical crosslinking. Lignin hydrogels have found applications in controlled drug release, wound healing, water treatment, agriculture, and smart biomaterials that could respond to stimuli. Lignin hydrogels has a long future but require more scientific inputs.

**Keywords:** Lignin, hydrogel, biopolymer.

## **Design of Multifunctional Biomaterials for the Application in Peripheral Nerve Regeneration**

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**Abstract:** Peripheral nerve injury (PNI) and its regeneration continues to remain a significant medical burden worldwide. The current treatment strategies used to treat PNI are often associated with multiple complications and yet do not achieve complete motor and sensory functions. Recently, synthetic biodegradable nerve conduits have become one the most commonly used conduits to repair small gaps in nerve injury. Even though synthetic conduits are cost effective and are associated with far less complications, in terms of nerve regeneration have not shown better results than nerve grafts possibly because of the lack of biological microenvironment required for axonal growth. Schwann cells which are functional glial cells of the peripheral nervous system, play a very crucial role in peripheral nerve regeneration where activated SCs produce multiple neurotrophic factors that help in remyelination and immune modulation during nerve repair. Studies have shown that compared to conventional synthetic scaffolds, nanofibrous scaffolds have better bioactivity and more closely mimic the native structure of extracellular matrix (ECM). Therefore, the present study was focused on designing a nanofibrous scaffold that would cover the roles of both structural support for the cells that can promote action potential at the synapse and provide a microenvironment with biological cues for nerve growth and regeneration. Here we used decellularized Schwann cell ECM to coat on polycaprolactone-graphene oxide aligned and random nanofibrous scaffolds to assist in remyelination and regeneration of axons. This multifunctional scaffold would be a potential biomaterial to treat peripheral nerve injuries and promote regeneration.

**Keywords:** Peripheral nerve regeneration, Electrospinning, Polycaprolactone, Graphene Oxide, Schwann cells and Acellular matrices

## **Design and Characterization of Maltose Conjugated Poly-Caprolactone Nanofibrous Scaffolds for Uterine Tissue Regeneration**

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**Abstract:** Uterine anomalies are prevalent in women and the major treatment assisted to them is hysterectomy as donor availability is extremely low. To overcome this, engineering uterine myometrium smooth muscle tissue has become very important. Several studies have shown that Poly-caprolactone (PCL) nanofibers are very effective in engineering smooth muscles, as this type of scaffold have structural similarities to the extracellular matrices (ECM) of the cells. Here, we hypothesize that by electrospinning PCL nanofibers, they form a suitable scaffold for uterine tissue engineering. Later, they are surface modified by a two-step wet chemistry method. First step is aminolysis which introduces the primary amine groups on the PCL scaffolds, making them hydrophilic in nature. In the next step, maltose is conjugated to improve the cell adhesion and increase the viability of the scaffolds. This was confirmed by Ninhydrin assay where the presence of amine groups was confirmed. This was followed by ELLA assay where the presence of maltose on the scaffold was quantified. Modified scaffolds were further characterized by various methods such as scanning electron microscope (SEM), contact angle analysis and Fourier Transform Infrared spectroscopy (FTIR). MTT assay and live-dead assay were performed on the maltose immobilization to study the improvement of the cell attachment and proliferation rates on the modified scaffolds.

**Keywords:** Poly-caprolactone, Nanofibers, Electrospinning, Maltose, Uterine tissue Engineering.

## NANOTECHNOLOGY AND DRUG DELIVERY

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**Abstract:** Lignin is a complex, amorphous, amphiphilic polymer. The second-most abundant organic polymer on earth after cellulose, it is a cross-linking irregular biopolymer. Lignin types - Kraft lignin reportedly acts as fat adsorbent, prevents obesity; alkali lignin reportedly shows antioxidant, antidiabetic properties (anti-hyperglycemic) and  $\alpha$ -amylase inhibitory activities (For instance, alkali lignin extracted from the deciduous plant *Acacia nilotica* shows antioxidant and antidiabetic characteristics); sulfated low-molecular weight lignin reportedly acts as an anticoagulant and immunomodulatory mediator. Lignin can also be employed in preparation of nanoparticles (NPs) which further find their diverse applications in drug administration system and also in anti-cancer treatment. It encompasses drug coating by a lignin nanoparticle carrier (drug encapsulation), drug administration into the body using appropriate routes of delivery (*in vitro* release and cellular uptake) and then deciphering the responses shown by the administered drug (in context of drug delivery and cancer therapy).

The synthesis of LNPs has been a recent development in lignin valorization. NPs have been observed acting as sunscreen antioxidants, free-radical scavengers, etc., but their role in controlled release drug delivery has been relatively low (reportedly). LNPs have potential applications in the biomedical and environmental fields, such as tissue engineering or regeneration, strong underwater antifouling materials. Numerous reports have shown the capacity of lignin-based NPs for the controlled drug release which are important in medicine. NPs synthesized from lignin are relatively non-toxic, highly biodegradable, stable and inexpensive; these four major advantages embody them as potent drug delivery systems in human diseases. Recently, water-dispersed lignin NPs have been made to carry silver ions ( $\text{Ag}^+$ ), which are significant in antimicrobial applications and/or in cancer treatments. Additionally, lignin is appropriate for transferring both hydrophobic and hydrophilic drugs. For instance, the pH-sensitive polymers are added to lignin NPs for facilitating easier loading of hydrophilic drugs. Poorly water-soluble drugs or water-soluble anticancer drugs

can be loaded on lignin NPs, leading to an increase in their anticancer and growth inhibitory effects in different cancer cell lines.

**Keywords:** Lignin nanoparticles, drug encapsulation, lignin valorization, biomedical applications, cancer.

### **SNP analysis and Basic characterization of gene SLC20A1**

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**Abstract:** In this study, analysis of missense SNPs and web-based characterization of gene SLC20A1 is carried out. Solute carrier family 20 member 1, SLC20A1 gene with GeneID 6574, has 394 missense SNPs listed in NCBI. The protein encoded by this gene is a sodium-phosphate symporter. Missense SNPs were analysed with online tools provean, polyphen 2 and panther to identify mutations which are deleterious. 87 SNPs were found to be deleterious by Provean, Panther and Polyphen 2. Panther, which utilizes position-specific evolutionary preservation, listed 259 of 394 SNPs as probably damaging with a false positive rate of ~0.2. Only 53 mutations were listed as benign by Panther. Provean showed that 130 are deleterious mutations. Polyphen 2 listed 151 snps as probably damaging. GeneMANIA showed that genes SLC20A2, PIGT, ATF1, CREB1, AP3D1, RAPGEF1, BZW1, STX2, PHLDA1, SLC25A32, UGT1A6, UGDH, MAP4K4, PIM3, NETO2, HSD17B2, IER3, LRRC8A, BARD1 and LMBR1L are related to SLC20A1. Pathway Commons which visualize interactions between genes shows that ATF1, CREB1, SLC20A2 and RAPGEF1 are coming into interactions with gene SLC20A1. Analysis of slc20a1 in STRING gave a network of proteins having 11 nodes and 14 edges, and with PPI enrichment p-value 0.154. Ten proteins which were found in the network are tnfrsf10b, slc37a4, lin7a, mpp2, mpp6, fech, slc34a1, rad1, rad51b and slc34a3. The network has an average node degree of 2.55 and average local

clustering coefficient 0.917. Six molecular functions (GO terms) were significantly enriched in the network, of which, phosphate ion transmembrane transporter activity has the highest enrichment effect of 2.74 ( $p = 1.19 \times 10^{-8}$ ) and protein domain specific binding has least enrichment effect 0.88 ( $p = 0.0278$ ). The cellular components (GO terms) enriched in the network are brush border membrane and cell projection membrane ( $p = <0.05$ ). Ten pathways (Reactome 2016) were enriched by Enrichr, in the analysis of above said set of 21 genes from geneMANIA and they are sodium-coupled phosphate cotransport, CREB phosphorylation, glucuronidation, nuclear events - kinase and transcription factor activation, MAPK targets/nuclear events mediated by MAP kinases, NGF signalling via TRKA from plasma membrane, signalling by NGF, MAP kinase activation in TLR cascade, TRAF6 mediated induction of proinflammatory cytokines and TLR10 cascade ( $p = <0.05$ ). The basic information gathered regarding SLC20A1 gene and protein would be integral in omics study of genetic disorders associated with kidneys because of its implications in urinary tract development.

**Keywords:** SLC20A1, SNP, missense, urinary tract development

## A Powerful Sword to Fight Bacterial Infections-Type III Secretion System

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**Abstract:** The emergence and rapid development of multiple drug-resistant bacterial strains present a major challenge to global public health. This encourages research professionals to look for unique clinical targets. The most prominent one is the **Type III Secretion System (T3SS)** found in nearly all gram-negative pathogenic bacteria. It is an effective needle-syringe mechanism, made up of more than 20 proteins and its pathogenicity can be eliminated by disruption of any component. The study aims to obstruct the **Tip Complex (TC)** of the T3SS system of *Salmonella sp.*, which is essential for host-bacteria contact, making it an excellent molecular target. This attachment is mediated by **SipD (Salmonella Invasion Protein)**. The objective was to target SipD using a Single Domain Antibody-mediated approach by integrating computational biology and recombinant DNA technology. Using *In Silico* tools, binding of the antigen-antibody complex was enhanced by introducing site-directed mutagenesis, Haddock Score (Docking Score) increased by 41.9%, and binding affinities ( $\Delta G$ ) and dissociation constant ( $K_d$ ) of docked complexes increased by 20% and 18% respectively. Affinity maturation via in silico mutagenesis is a key aspect of antibody engineering before in-vitro experiments. An optimized anti-SipD sequence was successfully cloned in expression vector-pET-39(b) followed by the characterization of the clone and expression of the anti-SipD protein (Mol. Wt. 14.89 KDa). Future work focuses on purification and molecular tests like ELISA to check the binding efficiency of an antigen-antibody complex. This approach can also be applied to other major disease models.

**Keywords:** Type III secretion system, tip complex, sipD.

## **Affinity maturation of single domain anti-CdtB antibody against *Salmonella typhi***

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**Abstract:** The main causative agent of enteric fever, *Salmonella typhi*, leads to 161000 deaths annually throughout the world. It is a human-restricted pathogen that possess a huge burden on developing nations like India. The cure of any disease starts with accurate and timely diagnosis, however, most tests currently available in the market lack reliability, sensitivity, accuracy, and specificity. The chances of cross-reactivity, as well as false positives, are also high. This inefficient diagnostic regimen signifies the dire need for precise, cheap, and more-reliable biomarkers to detect *S. typhi* infections. The B subunit of Cytolethal distending toxin has been recognized as an ideal diagnostic candidate, owing to its high specificity, immunogenicity, and expression only after *S. typhi*-infections. Our study aimed at generating an anti-CdtB antibody against the CdtB subunit of *Salmonella typhi* via *in silico* approaches. Affinity maturation of eight single domain antibodies was performed to calculate binding efficacy of anti-CdtB with the F chain of typhoid toxin (that encodes the CdtB subunit of *S. typhi*), using the modeling and molecular docking studies. *In silico* site-directed mutagenesis and macromolecular interface studies were performed to improve Ab-Ag binding and out of 248 mutated sequences, the sequence named 8AB63 exhibited the highest binding affinity towards the CdtB antigen of *S. typhi*. We further report cloning and expression of 8AB63 anti-CdtB protein in pET 39(b) expression vector. The future aim of this study includes purification of anti-CdtB protein and *in vivo* testing of *Salmonella typhi* infections using the anti-CdtB antibody.

**Keywords:** *S. typhi* diagnosis, CdtB, typhoid toxin, single-domain antibody, Ab-Ag docking, *In Silico* mutagenesis, anti-CdtB antibody.

**Molecular and Morphometric Characteristics of *Zea mays* Derived Xylanase Producing Fungi: Comparison of the Internal Transcribed Spacer (ITS) with Homologous Clinical Isolates**

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**Abstract:** Purpose. Fungi offer a rich source of biotechnological and therapeutic compounds unmatched by synthetic medicines. Innovative bioprocesses have been possible using fungal derived reagents owing to their extreme biodiverse characteristics. The purpose of this study is to explore the molecular landscape of the ITS (internal transcribed spacer) rRNA gene among xylanase producing environmental isolates and compare with the ITS of clinical pathogen isolates. Methods. Isolates were obtained from medium enriched with xylan and corn cob after several cycles. Ribosomal rDNA was analyzed by ITS (internal transcribed spacer) sequencing using ITS1 / ITS4 primer pairs. We searched a total 53 homologous ITS sequences from the ISHAM database for morphometric analysis. Hybrid secondary structures were modeled using RNAalifold. CRISPR sites were mapped in the ITS sequence using insilico for on-site target, microhomology prediction (CRISPR RGEN) and Blast CRISPR. Recombination with a multiple change point model allows across sites in multiple alignment. Results. The ITS secondary structures markedly differ from ISHAM homologous structures with extra stems, loops and bulges or a remodel polymorphism and exhibited a lowering of the minimum free energy (MFE) and free energy of thermodynamic ensemble. Microhomology and CCTop predictors tend to locate more sites towards half of the 3' end, while CRISP direct located more sites in the proximal 5' end of the ITS. Conclusion. The secondary structure of ITS rRNA differ from the clinical isolates and generally exhibited a more negative minimal free energy. The presence of potential CRISPR sites as well as recombination could provide versatile diversity.

**Keywords:** Xylanase, ITS rRNA, CRISPR, recombination.

**Biofortification of Seed by biotechnologically modified Nanoparticles: An easy and great way to improve malnutrition**

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**Abstract:** Micronutrient inadequacies in worldwide natural pecking orders are a huge reason for medical disease around the globe, especially in non-industrial nations. Agriculture is the essential wellspring of supplements needed for sound health, and as the population has kept on developing, the farming area has felt obligated to improve crop creation, as far as both amount and quality, to satisfy the worldwide needs for food security. The utilization of Biotechnologically Modified Nanoparticles (BMN) has arisen as a promising innovation to economically improve the effectiveness of current agrarian practices just as generally speaking crop profitability. One promising methodology that has started to get consideration is to utilize BMN as seed medicines to biofortify agrarian yield creation and quality. This audit features the present status of the science for this methodology just as basic information holes and exploration needs that must be defeated to enhance the manageable utilization of nano empowered seed fortress attractions near.

**Keywords:** Biotechnologically Modified Nanoparticles, Micronutrient inadequacies, and biofortify.

## **Naringin mitigates PTZ-induced kindling by modulating Dopamine, GABA and Glutamate in experimentally kindled mice**

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**Abstract:** Several mechanisms have been proposed for the development of epilepsy like disturbed ionic conductance, imbalance between inhibitory and excitatory neurotransmitters in addition to other theories. Naringin (flavanone-7-O-glycoside), a natural occurring flavonoid molecule, is considered by its effective neuromodulating properties. Accordingly, the objectives of the present study were to investigate its potential neuroprotective effect in experimental model of epilepsy. The kindling model was established by intraperitoneal (i.p.) administration of subconvulsive dose (25 mg/kg) of chemoconvulsant, pentylenetetrazole (PTZ). Animals were treated with naringin (40 and 80 mg/kg, p.o.) to study its probable antiseizure effect and mechanism. Mean seizure scores were assessed on every 7<sup>th</sup>, 14<sup>th</sup>, 21<sup>st</sup>, 28<sup>th</sup> and 35<sup>th</sup> day of dosing. The levels of dopamine, GABA (gamma-aminobutyric acid) and glutamate in the hippocampus and cortex of experimental mice were assessed using ELISA Technique. Naringin treatments displayed significant decrease in seizure scores in kindled mice in a dose-dependent manner. Furthermore, the naringin administration was able to modulate the levels of neurotransmitters in the hippocampus and cortex of kindled mice. Our findings suggest a therapeutic potential of naringin against seizure severity by restoring the levels of neurotransmitters during PTZ-induced kindling in hippocampus and cortex of kindled mice.

**Keywords:** Naringin, pentylenetetrazole, GABA, glutamate, dopamine, kindling

**Detection of Pharmaceutically Significant Homoisoflavanoid Bonducellin through LCMS in an Ethnomedicinal Plant - *Caesalpinia bonducella* (L.) Roxb.**

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**Abstract:** The objective of the present study is to detect the presence of homoisoflavanoid – bonducellin in *Caesalpinia bonducella* (L) Roxb. Ethanolic extract of in vivo and in vitro plant materials – different plant organs, developmental stages and callus obtained from leaf explant of *Caesalpinia bonducella* (L) Roxb. on MS medium supplemented with 1mg/l and 2 mg/l 2,4-D, 1mg/l NAA and 4mg/l BA were subjected to LCMS for the detection of bonducellin. Plant organs – seed kernel and seed coat, developmental stages – shoot at flowering, shoot after flowering, 30 days old seedling plant, 60 days old seedling plant, 90 days old seedling plant and 120 days old seedling plant were found to contain bonducellin. The bonducellin was absent in plant organs – root, stem, leaf, pod and developmental stage shoot before flowering in *Caesalpinia bonducella* (L) Roxb. Detection of bonducellin in ethanolic extract of *Caesalpinia bonducella* (L) Roxb. will help to select the most appropriate plant organ for the extraction of bonducellin. Our study also provides an alternative method for the extraction of bonducellin through callus culture which can be used in future for large scale production of bonducellin without disturbing the natural population of the critically endangered plant - *Caesalpinia bonducella* (L.) Roxb.

**Keywords:** Bonducellin, *Caesalpinia bonducella* (L.) Roxb, LCMS, in vivo, in vitro developmental stages, homoisoflavanoid.

## **An Overview on Awareness on Use of Medical Devices in Management of Non-Communicable Diseases in Rural and Urban Areas of Kadapa**

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### **Abstract:**

**Background:** Today, the incidence of Non-Communicable Diseases (NCDs) were ubiquitous and were observed in every nook and corner of the world and these should not be neglected as they deteriorate the Homo sapiens.

**Aim & Methods:** To monitor the knowledge in usage of medical devices for NCDs in rural to urban settings of Kadapa, Andhra Pradesh and this was a prospective observational study conducted for 1.5 years.

**Results:** Subjects (n = 1024; urban (n = 438 (42.77%)), rural (n = 586 (57.22%))) were recruited and 54.68% (n = 560) of subjects were male and 45.31% (n = 464) subjects were female; 73.92% (n = 757) of subjects were literates and 26.07% (n = 267) subjects were illiterates. Various occupational status of subjects includes that 67.38% (n = 690) of them were daily wage labors, 14.64% (n = 150) of subjects were farmers, 9.76% (n = 100) of subjects were domestic engineers and 8.20% (n = 84) subjects belongs to various other occupations. Different NCDs in recruited subjects were diabetic and hypertensive subjects constitute 70.70% (n = 724), diabetic and thyroid subjects constitute 8.78 % (n = 90), other pathological conditions constitute about 20.50 % (n = 210). In urban and rural areas awareness on the use of medical devices was seen among 327 (31.93%) and 193 (18.84%) subjects, respectively.

**Conclusion:** From findings, it was observed that knowledge in the usage of medical devices was higher in urban areas.

**Keywords:** Non-Communicable Diseases, rural and urban areas, medical device, educational status.

## **Pattern of acephate tolerance in bacteria isolated from the surface of grape berry**

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**Abstract:** Acephate is an organophosphorus pesticide which has no label claim for grapes. It is registered in India for use in different crops. It is however sometimes detected in grapes from direct or indirect source. The microbes of grape berry, in which there is a chance contamination by acephate, get exposed to this pesticide. It would be interesting to see whether the resident microflora is able to tolerate and degrade acephate. Usually, microorganisms isolated from the pesticide contaminated site have the ability to degrade the pesticide. In this study we report that the grape berry harbors microorganisms that have the ability to tolerate this pesticide but is unable to degrade them. This ability of the microbes to tolerate acephate and inability to degrade it can be related to its possible residues in grapes.

**Keywords:** grape, epiphytic microbe, pesticide tolerance, residues in grapes, plant protection.

## **A selective and sensitive immunosensor for the detection of pathogens based on CuO-ZnO nanocomposite**

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**Abstract:** The present study reports the synthesis of CuO-ZnO composite by a solution combustion method using polysaccharide as a template. Synthesized ZnO and CuO-ZnO composites were characterized using XRD, SEM, EDX, and FTIR analysis. The SEM analysis showed the formation of spherical nanoparticles with the average size of 40-70 nm. Further, a facile electrochemical immunosensor based on CuO-ZnO nanocomposite modified Screen Printed carbon electrode (SPCE) was developed for sensitive detection of *S. aureus* and *E. coli*. The electrochemical behavior of CuO-ZnO composite and antibody conjugated CuO-ZnO nanocomposite modified SPCE was studied. It was found that the cumulative effect of CuO and ZnO leads to the enhancement in the sensing response towards the bacterial pathogens. The CuO-ZnO nanocomposite based immunosensor could detect *S. aureus* in a linear range of 1-10 cfu/ml. The developed sensing method doesn't need sample preparation and processing and the extraction of the sample. This immunosensor can be further explored for its usefulness in real-time analysis of bacterial pathogens, considering the need for early detection.

**Keywords:** Nanocomposite, metal oxides, pathogens, electrochemical, immunosensor

## **Lifestyle and Dietary factors causing Microsatellite Instability Gastric Cancer detected using Ensemble modeling**

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**Abstract:** This retrospective cohort study focuses on supervised machine learning (ML) techniques for identifying diet and lifestyle patterns that cause microsatellite instability gastric cancer (MSI-GC). There were 142 genetic variants acquired via targeted resequencing of 60 biomarker genes from gastric tumor samples and tabulated with respect to MSI status, diet and lifestyle characteristics. Learning curves and feature selection methods were devised to choose the best algorithms, to reduce the complexity of heterogeneous data and to key out the features of importance. Data analysis revealed features extracted using ridge regression and extra salt, smoked food, smokeless tobacco products (Khaini / sadha), alcohol and betel nut leaf with lime (khuva) were the core factors for causing MSI-GC. The features set was exploited using random forest and multilayer perceptron classifiers with 96% accuracy, precision, recall, F1 score, and Receiver operating characteristics (ROC) curve which is a well-balanced classification score. The brier score was 0.04 and Matthews correlation coefficient (MCC) was +0.91. These features show excellent performance for both random forest ensemble classifier and multilayer perceptron back-propagation classifier which further strengthens the extracted features (risk factors for MSI-GC). Based on the integration of mutation and diet-lifestyle data using ML, this is the first time report that demonstrates that extra salt, smoked

food, Khaini / sadha, alcohol and khuva are the major diet and lifestyle risk factors causing microsatellite instability gastric cancer.

**Keywords:** Microsatellite instability gastric cancer (MSI-GC), Matthews correlation coefficient (MCC), brier score, exome data, diet, lifestyle, supervised learning algorithms.

**Biosynthesis of Selenium Nanoparticles from *Paenibacillus* sp. and its Functionalization with Nystatin for Improved anti-biofilm activity against *C.albicans*.**

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**Abstract:** Among total infections caused by *C.albicans*, 90% involve biofilm formation, biofilms are resistant to existing antibiotic therapy. The major problem associated with antibiotics such as Nystatin is drug resistance developed by *C.albicans* resulting in the necessity for alternative or combinatorial therapy to treat resistant *C.albicans* sp. incorporation of antifungal drug Nystatin into a Nano-carrier can increase the bioavailability of Nystatin and can increase its efficacy at lower dose concentration. Nanoparticles can be used as a smart drug vehicle by either encapsulating or by attaching it to the antifungal agent through nanofabrication or functionalization with various biocompatible synthetic polymers. Selenium nanoparticles are not only used as a food additive especially in individuals with selenium deficiency, but they can also safely used as a medicine or as a drug carrier with higher degradability, lower toxicity, and gradual clearance from the body without significant side effect. In the present study, we biosynthesized SeNP from *Paenibacillus* sp. and studied the Anti-biofilm activity of SeNP functionalized with Nystatin in *C.albicans*. The

mechanism of inhibition of *C.albicans* biofilm was studied by using the RT-PCR approach by quantifying the fold expression of the genes which play a pivotal role in the morphogenesis of *C.albicans* and the formation of biofilm. Finally, the cytotoxicity of Nystatin functionalized SeNP on a normal cell line was studied. Overall this study explains the use of SeNP as a smart drug carrier to increase the efficacy and bioavailability of Nystatin against *C.albicans*.

**Keywords:** SeNP, *Paenibacillus*, Nystatin, anti Biofilm, *C.albicans*, qRT-PCR.

# ***Poster Presentations***



### **Treating cancer with nanorobots**

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**Abstract:** Nanorobotics is an emerging field of nanotechnology which deals with design and construction of devices at nano level which is extremely small to transverse inside the human blood. Application of nanorobots in the treatment of cancer is one of the fascinating fields of research. The current techniques for cancer such as chemotherapy and radiotherapy are not specific to cancer cells and do affect healthy cells too. Nanorobots which are roughly 100 times smaller than human tissue, is made from a flat, rectangular DNA origami sheet, 90 nanometers by 60 nanometers in size. The key to programming a nanorobot that exactly attacks a cancer cell was to include a DNA aptamer (short nucleotide strands with special sequences for recognizing target cell). The drug is loaded inside the nanorobot, and it is secured by molecular anchors. The aptamers act as clasps, and once they recognize their target, the device opens up and releases the payload(drug).Each nanobot was labeled with fluorescent markers, to analyze how and where the drug has been delivered. Nanorobots deliver thrombin, an enzyme which clots the blood that goes to the tumor, thereby blocks blood flow to tumor cells, causing a sort of mini tumor attack, and leading to tumor tissue death. Speed, durability and controlled release of drug specific to cancer are its dominance. Drawbacks are expensive and research work has to be done for the robots to overcome the body's immune response.

**Keywords:** nanotechnology, cancer, nanorobots, DNA aptamer, fluorescent, thrombin

### **Biosensor for the Detection of Bird Flu**

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**Abstract:** The avian influenza viruses (AIVs) are highly infectious, causing the bird flu which leads to the health, social problems to the human beings. The idea of this poster is to develop a biosensor for the rapid detection of avian influenza virus (AIV) for both the birds as well as for the humans using a single detection kit. The poster focuses mainly on the working principles and its application for the virus detection in these organisms by using the biosensor technology and to discuss important aspects for developing biosensor which can quickly detect the presence of AIVs in humans as well as birds. The main motive behind this idea is to get the AIVs tested in both the organisms using the same kit with ease. Unlike the existing testing methods, the idea is to make it user friendly and cost effective. Hence, opening a way for the development of a highly sensitive biosensor for the rapid detection of AIV in both humans and birds, which reduces the health, economic, and social impact caused by this virus.

**Keywords:** AIVs, biosensor, work flow, sensor strip, flow direction, bioreceptor.

**A study on the gene alterations in putative calcineurin substrates in leukemia, based on cBioportal database.**

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**Abstract:** Calcineurin (CaN) is a calcium/calmodulin dependent Ser/Thr phosphatase which plays a crucial role in intracellular signaling. Studies on the calcineurin signaling have demonstrated its role in cell proliferation, cell migration and metastasis. Several putative substrates that undergo dephosphorylation include transcription factors, cytoskeletal proteins, apoptotic and cell cycle proteins, scaffold proteins and ion channels. The present study is an attempt to query these substrates for the mutations in acute lymphoid leukemia and acute myeloid leukemia using the cBioportal database. Preliminary analysis of the data from cBioportal database showed that out of the two genes that were queried (CXCR4 and MAP2), MAP2 had a missense mutation in 0.6% of acute myeloid leukemia cases. These two genes did not demonstrate any mutations in acute lymphoid leukemia. Further analysis of other genes and a comparative profile of the changes in the calcineurin substrates will be discussed herewith.

**Keywords:** Calcineurin, CXCR4, MAP2, leukemia.

**Human Serum Albumin as a nanocarrier for the efficient delivery of Piperlongumine: Preparation, Characterization and *In vitro* studies.**

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**Abstract:** Piperlongumine (PL), is a small natural biologically active alkaloid that exhibits anti-inflammatory, antibacterial, antifungal, antidiabetic, antiatherosclerotic and anticancer activity. In recent years, PL has gained increasing interest as a potential anticancer drug but poor water solubility and low bioavailability limits its clinical use for cancer treatment. Hence, to overcome these limitations and enhance its anticancer activity, we formulated PL loaded Human Serum Albumin (HSA) nanoparticles by desolvation method. HSA nanoparticles has been explored for their clinical applications due to its bioavailability, biodegradability, low toxicity and non-immunogenicity. Thus, we consider HSA as a nanocarrier to encapsulate PL for delivery and enhanced anticancer efficacy. HR-TEM images implied that the nanoparticles are of spherical shape. The FT-IR spectra, XRD patterns and DSC thermograms confirmed the encapsulation of PL in amorphous form in HSA nanoparticles. Stability studies suggested that PL remained stable up to 3 months in different buffers. *In Vitro* drug release studies suggests controlled and sustained release. The cellular uptake study proved that PL successfully deliver at its target sites and further EtBr staining suggests that HSA nanoparticles are more effective and enhanced the anticancer activity of PL as a therapeutic agent. *In vitro* cytotoxic studies and colony formation assay proved that PL loaded HSA nanoparticles are more toxic towards colorectal cancer cells and kill more cells as compared to pure PL. In summary, PL loaded HSA nanoparticles as drug delivery system could be clinically effective for colorectal cancer.

**Keywords:** Cancer, Human Serum Albumin, Nanoparticles, Drug, Biocompatible

**Photocatalytic degradation of Dyes using metal Nanoparticles synthesized with *Piper betel* (Betel) leaf extract and Fructose as Reducing agents**

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**Abstract:** In India, textile industry is the second largest employment generating sector. Approximately 10,000 different dyes are used, but 200,000 tons of dyes are lost as effluent every year during dyeing and finishing operations. Dyes from effluents escape conventional wastewater treatment processes and persist in the environment due to their high stability to light, temperature, water, detergents, chemical soaps and other parameters. The aim of this study was to synthesize and characterize nanoparticles using different metals in presence of betel leaf extracts and fructose as reducing agents and also to determine their photocatalytic efficiency in degradation of dyes. The results indicated, the formation of metal nanoparticles that was confirmed using UV-Vis Spectrophotometer. Particle sizes were analysed using SEM. FTIR spectra with wave numbers showing sharp peaks at 3524.06 cm<sup>-1</sup>, 1641.48 cm<sup>-1</sup>, 3460 cm<sup>-1</sup>, 1631.83 cm<sup>-1</sup>, 3444.98 cm<sup>-1</sup>, 1527.67 cm<sup>-1</sup>, 3583.86 cm<sup>-1</sup>, 1666.5 cm<sup>-1</sup> obtained might be due to various functional groups of phytochemicals of betel leaf extract, fructose and metal ions. XRD powder analysis showed that zinc nanoparticles were pure with particle size 30.1 nm, copper oxide and copper nanoparticles were 52 nm and 49 nm respectively. Characterized nanoparticles were treated with dyes and exposed to sunlight for six hours for photocatalysis. The results showed that, the catalytic efficiency of copper nanoparticles had maximum degradation on all the dyes when compared to other metal nanoparticles. Degradation of dyes using biologically synthesized nanoparticles would be a simple, rapid and convenient method to minimize harmful dyes accumulation and can be implemented and scaled up nationwide.

**Keywords:** Betel leaf, dye degradation, FTIR, nanoparticles, photocatalysis, SEM, XRD.

## REGENERATION

Surabhi Awasthi

**Abstract:** Regeneration itself is a very interesting word since 4<sup>th</sup> Century. It will surprise you that stem cell therapy originated from the birth of 100 kauravas. Idea of regeneration is as old as humanity. Organisms can regenerate their body parts in different ways. Some animals can replace their missing parts by first growing a blastema such as Jelly Fish. The Mass of cells (blastema) has the capability to divide and form the skin, scales, muscles, for creating the lost limb or tail.

Loss of organ by birth or sometimes due to infections or diseases, can compromise the quality of life of an individual. Now-a-days, Medical field is focussing on non-functional cells or restoring the function of an impaired organ. For achieving the objects in regenerative therapy which includes mesenchymal, hematopoietic, embryonic and induced pluripotent stem cells etc. Recent Advances in tissue regeneration and the Application of Stem cell transplants are treating many life threatening diseases or improving the quality of life.

**Keywords:** Regeneration, Stem cells, Tissue engineering, Blastema.

## **Synthesis and analysis of Zinc Oxide Nanoparticles in presence and absence of *Ocimum Sanctum* leaf extract**

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**Abstract:** Green synthesis of nanoparticles from biological systems especially from plant extracts have become an emerging field in nanotechnology. In this study, zinc oxide nanoparticles were synthesised by using zinc nitrate as precursor. The main objective of study was to reduce size of zinc oxide nanoparticles by using a capping agent and make it as biosafety material. Aqueous extracts of capping agent *Ocimum sanctum* were used along with two different concentrations of zinc nitrate (0.05M and 1M). Control samples were also made in absence of leaf extract. The synthesized nanoparticles were characterized by UV-Visible and X-Ray Diffraction analysis (XRD). UV-Vis spectra showed typical absorption peak at around 363 nm, which is in the standard range (330 nm-460 nm), suggested the formation of Zinc Oxide (ZnO) nanoparticles. X-ray diffraction analysis was done and size of particles was calculated using Scherrer equation. The average size of the zinc oxide nanoparticles synthesized from 0.05M zinc nitrate (control-absence of leaf extract), 0.05M zinc nitrate and 1M zinc nitrate (test-using leaf extract) were found to be 26nm, 23nm, 33nm respectively. The ZnO nanoparticles formed at 0.05M zinc nitrate and in presence of capping agent (*Ocimum sanctum* leaf extract) was relatively smaller in size compared to other preparations tested. This study clearly indicates that appropriate concentration of Zinc nitrate solution and presence of capping agent are very useful in preparing small size of nanoparticles and can be used as biomaterial for various applications in medicine and other areas.

**Keywords:** Zinc nanoparticles, *Ocimum sanctum*, XRD-analysis.

## **A Digital Survey on the Acceptance and Affordability of COVID 19 Vaccine among the People of West Bengal, India- A Survey Based Study**

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**Abstract: Overview:** Currently, multiple vaccines for coronavirus disease 2019 (COVID-19) are in clinical trials. In Oct-Nov 2020, 1078 individuals in West Bengal surveyed to evaluate possible acceptance rates, affordability and factors affecting the acceptance of a vaccine for COVID-19.

**Method of Study:** The google form is prepared with the questions on acceptance and affordability of vaccines. The form is circulated digitally among the people and then we have collected the data in excel. Based on the result we have prepared our statistical graphs.

**Result:** 77.27 percent of respondents reported that they would be very or very likely to take a vaccine for COVID-19, 5.3 percent don't want to take vaccine and 12.24 don't know about their decision. In that 58 percent respondents want to take Indian Vaccine; 19 percent respondents want to take foreign vaccine. Other respondents can take any vaccine. The affordability, 40 percent respondents want a vaccine bellow 500 INR, 25 percent respondents want a vaccine of 500-1000 INR. 11 percent respondents want vaccine of over 1000 INR.

**Conclusion:** Majority of Responders want a COVID 19 vaccine. Majority responders want Indian COVID19 Vaccine. Majority responders want a vaccine in a cost of below 500 INR.

**Key Words:** COVID19, Vaccine, Acceptance, Affordability

### **Nanofertilizers and their delivery system: A boon to agriculture**

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**Abstract:** India is an agriculturally based country. 30-40% of crop productivity in the agriculture depends on the fertilizers. The use of conventional fertilizers has led to reduction in soil fertility, low productivity and pollution to environment. Nanotechnology offers a promising future in providing sustainable agriculture. Nanofertilizers improves the quality of soil, stimulate plant growth and overall productivity in terms of plant yield. Nanofertilizers have potential to increase crop productivity through slow and controlled delivery. Nanofertilizers improve the bioavailability of nutrients owing to high specific surface area, mini size and more reactivity. Nanoparticles with their small size and target specificity can deliver nutrients to specific target sites in plants. The delivery of nutrients to crops can be done by encapsulating nutrient inside a nanomaterial such as a nanotube, coating with a thin protective film or through attachment on nanoparticles using ligands. Impact and efficiency of nanofertilizer on the plant system depends on the method of application. Various methods of application of nanofertilizers to the plants like hydroponics (in vitro) and foliar application (in vivo) can be used. Nanofertilizers hold a great potential to boost the agricultural output at the desired rate when used in optimum concentrations while overcoming the limitations of conventional fertilizers.

**Keywords:** Nanobiotechnology, nanofertilizers, agriculture, bioavailability, encapsulation

**Cartap hydrochloride induced stress response in *Anabaena variabilis* ARM 441**

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**Abstract:** Cartap hydrochloride is a moderately hazardous nereistoxin analogue insecticide that is deliberately applied in paddy fields of India, at a recommended dose of 10  $\mu\text{g ml}^{-1}$  to kill chewing and sucking insect pest of rice crop. Cartap toxicity was studied on non-target free-living nitrogen fixing algal biofertilizer cyanobacterium *Anabaena variabilis* ARM 441 commonly used in rice cultivation. *Anabaena sp.* could tolerate commercial grade insecticide upto 30  $\mu\text{g mL}^{-1}$ . However, at the recommended dose it reduced algal growth by 30.93 in 5  $\mu\text{g ml}^{-1}$ , 57.31 in 10  $\mu\text{g ml}^{-1}$  and 96.99 % in 20  $\mu\text{g ml}^{-1}$  as compared to control cultures. Cartap hydrochloride induces stress, since level of superoxide dismutase, peroxidase and catalase were also increased. Generation of superoxide radicals and hydrogen peroxide were increased by 152.48 and 34 % respectively. There was also increase in lipid peroxidation by 31.03 %. There was decline in ascorbate content by 48.45 %, however the glutathione content was increased by 128.57 %. Osmolytes such as proline was increased from 8.6-32.8 % and sucrose from 61.22-90.13%. Scanning electron micrographs revealed cell rupture and breakage in filaments due to cartap exposure with the formation of akinetes. The study indicates possible role of osmolytes in overcoming cartap stress and can be helpful in assessing detrimental effect on paddy field cyanobacteria, as cyanobacteria are purposely used as biofertilizers and nitrogen contributors in paddy fields.

**Keywords:** Cyanobacterium, cartap hydrochloride, antioxidant enzymes, osmolyte.

## **Preparation of cellulose derived silver nanogel and its implementation for heavy metal adsorption in industrial waste water**

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**Abstract:** Recently, development of materials based on biopolymers in sorption process for removal of heavy metal ions from wastewater has been considered by many researchers. The simplest, high efficiency and cheapness of an adsorption process make it most widely used among other processes. Numerous researchers had worked on the isolation of cellulose (popular carbohydrate polymer) from lignocellulosic biomass and utilization of cellulose based materials as effective adsorbents for the successful removal of heavy metals from wastewater. The sudden interest on cellulose and cellulose-based materials as adsorbents because of their excellent properties (biodegradability, renewability, economic value, biocompatibility, non-toxicity, high mechanical properties and surface area). Addition of silver nanoparticles on the nanogel increases the adsorption capacity as reported in various literatures. The nanogel and nanocomposite were characterized by various techniques (SEM, TEM, FTIR, XRD etc). Upon comparison with established adsorbents reported from various literatures, cellulose-based materials performed excellently well in the adsorption of heavy metals with Langmuir isotherm and pseudo-second order reported mostly (best fit models) for the generated equilibrium and kinetic data, respectively. It points at distribution of adsorption sites to be homogeneous as well as the formation of monolayer adsorbate on their surfaces. The various thermodynamic studies reported further, revealed the adsorption processes of heavy metals onto cellulose-based materials to be entropy driven processes, spontaneous, and endothermic. Finally, future research was suggested to focus on optimization to enhance the performance of the cellulose-based adsorbents, carrying out the adsorption on industrial wastewater as well as adsorbate which include contaminants such heavy metals.

**Keywords:** Cellulose, nanogel, wastewater, heavy metals, adsorption.

**Functional and regulatory aspects of X monosomy in response to oxidative stress.**

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**Abstract:** The partial/complete loss of one X chromosome lead to Turner Syndrome. The X-monosomy is regulated by genetic and epigenetic factors that may affect the cell behaviour. Thus, it is important to understand response of X monosomy to external stress which might contribute to various comorbidities in aneuploidy individuals.

We have performed RNA sequencing to reveal functionality associated with X monosomy under normal & mild oxidative stress. Our analysis showed significant differential expression of 814 genes (DEGs) in X-monosomy and 661 genes in response to oxidative stress. Further, gene ontology studies provide evidence that processes associated with bone metabolism, pregnancy, growth, and diabetes are altered in X monosomy.

Interestingly, pathways associated with oxidative stress are differentially expressed in X monosomy. We have therefore exposed 45, X and 46, XX cells to sub-lethal oxidative stress to understand the stress handling capacity of X monosomy cells. Surprisingly we found pathways upregulated in X monosomy under normal conditions showed downregulation after exposure to oxidative stress suggests different regulation of associated genes. To explore this we mapped transcription factors (TFs) in DEGs obtained from normal and oxidative stressed 45,X & 46,XX cells. We found differential expression of 63 & 60 TFs in X monosomy & oxidative stress respectively. Overall findings indicate that X monosomy cells are susceptible to oxidative stress compared to normal cells and have altered molecular pathways. Thus, study postulates that the altered ability of 45,X cells to respond to stress, may play a significant role in the physiological function and altered phenotypes in turner syndrome.

**Keywords:** Aneuploidy, Turner Syndrome, RNA-seq, oxidative stress, transcription factor.

**Synthesis of silver nanoparticle by the most radiation resistant bacteria  
*Deinococcus radiodurans* and its application as green nanophotocatalysts**

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**Abstract:** In this study, we report biogenic synthesis of silver nanoparticles (AgNPs) using polyextremophilic bacteria *Deinococcus radiodurans*. Optical and structural properties of the green synthesized silver nanoparticles was investigated by various techniques including Fourier transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), scanning electron microscopy (SEM), energy- dispersive X-ray (EDX) spectroscopy and UV –Vis absorption spectroscopy. In addition, the AgNPs entrapped in calcium alginate beads were used for photodecolorization of various charged pollutant dye, under solar irradiation. In this study, methylene blue, methyl orange and methyl green was selected as representative cationic and anionic dyes, respectively. AgNPs in the suspension as well as entrapped in beads could degrade all the three dyes. The photocatalytic activity of immobilized AgNP in fabricated column model shows potential application for removal of dyes from effluents contributing ultimately to ecological clear out process and facilitated in recovery and reprocess. The efficiency of beads entrapped silver nanoparticles as a promising candidate for the catalysis of organic dyes is established in the present study.

**Keywords:** Silver nanoparticle, *Deinococcus radiodurans*, green nanophotocatalyst, Azo dye degradation.

**Drug repurposing for treatment of SARS CoV-2 patients: an in silico analysis of HCV/HIV drugs against NSP12**

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**Abstract:** The novel coronavirus, also designated as Severe Acute Respiratory Syndrome Coronavirus 2 (SARS Cov-2) has created a global pandemic, resulting in loss of several lives. The world is still in the midst of the pandemic and there is an imminent need to develop better treatment modalities. Drug repurposing has gained significance in treatment of SARS CoV-2 because of the lower costs involved in development and shorter timelines. Studies have demonstrated a rapid growth in data related to structural proteins as druggable targets. With the evolution of mutation in structural proteins like the B117 strain, the focus for drug discovery and development have shifted towards the non-structural proteins (NSPs). In this work, we have performed the *in silico* docking of various drugs already used for the treatment of Hepatitis C virus and Human Immunodeficiency Virus against the RNA dependent RNA polymerase (RdRP) domain of NSP12. The amino acid sequences of the NSP12 protein of representative viral strains from across the globe were aligned to understand the conserved sites. The RdRP domain was also analysed for probable development of mutation. Several drugs that were used for the study gave good docking scores with NSP12 and it was predicted that a mutation was likely to develop at R750 of the NSP12. In this study, we iterate the significance of drug repurposing and using NSP12 as a target for treatment of SARS CoV-2 patients.

**Keywords:** SARS Cov-2, drug targets, non-structural proteins, NSP12, RdRP, mutations, drug repurposing.

**Evaluation and validation of QTLs clustered on chromosome 6 and chromosome 25 for pubescence in relation to jassid resistance in cotton (*Gossypium Spp.*)**

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**Abstract:** In cotton, among pests boll worms are the major concerns of yield loss. But in recent years Bt transgenic is one of the most promising technology to combat against these boll worms. Eventually which had reduced the number of sprays required to control the same. But as these Bt toxin acts more specifically to boll worms and with the reduced number of sprays, the other pests remain unaffected. Among these the sucking pests like jassid, which are secondary pests once has become the primary pests of concern in the Bt genotypes. Nevertheless it is well known that pubescence/hairiness on different parts of the plant can effectively avoid the attack by these sucking pests. Thus to keep the Bt genotypes unaffected from the sucking pests, it is necessary to incorporate the pubescence trait into the Bt background. Keeping this in mind in our study we have evaluated and validated 29 marker loci which are reported to be linked with pubescence traits in relation to degree of jassid resistance in cotton. These markers are found to be distributed among chromosome 6 and chromosome 25. Out of 29, 24 markers were found to be polymorphic among the parents. These 24 markers were used for genotyping of 306 F2 interspecific mapping population. By QTL analysis it is revealed that 22 markers were distributed among two linkage groups LG1 and LG2 which corresponds to chromosome 6 and 25 respectively. These 22 markers were found to be linked with pubescence, either with its density or its length. Out of these, eleven significant QTLs for pubescence were identified. Which can be effectively used to screen the Bt genotypes with pubescence background. Thus conventional breeding in association with molecular markers

can help in host plant resistance to provide a germplasm / cultivar base to achieve durable resistance to insect pests.

**Keywords:** Pubescence, QTLs, markers, linkage groups, Bt

### **Design of a UV Sanitization Unit in Powered Air Purifier Respirator (PAPR)**

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**Abstract:** The present work is related to the development of a Powered Air Purifying Respirators (PAPR) that is portable, with battery powered respirators and an inbuilt purifier that is used for supplying contaminant free air to the facepiece. As microorganisms of size less than 0.3 micron can pass through HEPA filter, to increase the disinfection efficiency of the air breathed by healthcare professional, we have designed and developed a prototype that includes a chamber to incorporate UV light in the PAPR system thereby increasing the irradiation efficiency to 4log. The devised design operates at 275nm UV-C with an intensity of 40.58 mW/cm<sup>2</sup> and is fitted after the HEPA chamber to attain uniform disinfection of microorganisms and is capable of sterilizing the continuous flowing air in about 1.3 secs. The parameters such as type and duration of exposure of UV light, air flow rate, dosage, amount of pathogen (log reduction) exiting the device, moisture and temperature are been considered while testing the model. Further details will be presented during the poster session of the conference.

**Keywords:** PAPR, irradiation, intensity, log reduction, HEPA, CAD, disinfection.

### **Exploring mangrove soil microbes for cellulolytic activity**

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**Abstract:** Mangrove sediment has a typical saline and humid weather conditions which harbors diverse microorganisms that are important for environmental bioremediation. Cellulose is one of the most abundant biomaterials on the earth. It is a linear and polydisperse polymer that consists of  $\beta$  -1, 4-linked glucosyl units. Cellulase is an enzyme that degrades cellulose and is produced by mesophilic microorganisms that is being used in various biotechnological processes. The enzyme synthesized is usually unstable in industrial environments, thus it is necessary to direct research towards cellulolytic microorganisms that can produce stable and active enzyme even under harsh physicochemical conditions. The aim of the present study is to carry out isolation, identification, characterization and screening of bacteria from mangrove soil and evaluate their cellulolytic potential by semi-quantitative screening method. The isolates were screened using carboxymethyl cellulose (CMC) plate assay and the zone of hydrolysis was obtained for positive isolates.

**Keywords:** Mangrove soil, bioremediation , cellulose, cellulase.

**A comprehensive study of classification models for ovarian cancer driver genes derived from functional analysis of mutations and driver gene interaction network**

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**Abstract:** Ovarian cancer (OC) is the most common type of gynecologic cancers in the world with a high rate of mortality. Mutation accumulation is the basis for cancer progression hence; identifying mutations in the driver genes is a key step in cancer diagnosis. Due to manifestation of generic symptoms and absence of specific biomarkers, the diagnosis of OC is usually done in the late stage. Thus, there is an imperative need for identifying potential biomarkers and drug targets from clinically significant gene mutations responsible for cancer. In order to understand cancer progression, different machine learning models are implemented in clinical practice. In the present study, a comprehensive analysis of whole exome sequences from 47 adult female OC patients was carried out to identify the mutations and generate functional analysis scores using Next Generation Sequencing (NGS) technique. A machine learning classification model was developed for predicting OC driver genes based on different functional analysis scores which yielded an accuracy of 89.35% (AUC value of 0.976). A driver gene interaction network was generated and analyzed to identify the relationship of novel driver genes with cancer associated pathways. The results were corroborated to reveal putative cancer driver genes that have potential implications in clinical diagnostics.

**Keywords:** Ovarian cancer, mutations, next generation sequencing, machine learning, driver genes, computational analysis.

## **Beneficiary effect of polyunsaturated fatty acids (PUFAs) in chemotherapy**

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**Abstract:** Dietary intake of polyunsaturated fatty acids (PUFA), like omega-3 and omega-6 PUFAs affect several immune functions in cancer. PUFAs are considered as Pharmacosupplements and are universally used as adjuvants in the cancer therapy due to their substantial biological effects on cancer. PUFAs have crucial role in cell- cell signalling, membrane composition, and intracellular pathways. Various preclinical studies as well as clinical trials suggest that PUFAs improve cytotoxic effects of several anticancer drugs. There are various mechanisms proposed to explain how omega-3 and omega-6 PUFA modulate the tumor cell response to chemotherapeutic drugs. After readily incorporation into cell membranes and lipid rafts, PUFAs affect many membrane-associated signalling proteins such as G- protein, ROS, RAS, Caspase, Akt. PUFAs increase apoptosis by altering expression or function of apoptotic proteins, or by modifying action of transcription factors such as nuclear factor- $\kappa$ B. Preclinical data reveals that PUFAs and their metabolites modulate underlying pathways which causes side effects of chemotherapy, indicating that this is a promising field of knowledge to be explored. Further research is necessary to identify specific mechanisms by which PUFAs increase chemotherapy efficacy and reduces side effects of chemotherapy. This critical review discusses about the effects and the possible underlying cellular/membrane level mechanisms of PUFAs supplementation for their betterment as adjuvants to chemotherapy.

**Keywords:** Polyunsaturated fatty acids (PUFA), Pharmacosupplements, cancer, chemotherapy

**Multi-omics approach for identifying oncogenic pathways associated with driver genes in Breast cancer**

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**Abstract:** The alterations in biological and molecular pathways can lead to oncogenesis factor. Identification of those pathways can be significant to study the pathogenic alterations mechanism which helps to develop potential therapeutic targets for cancer. Study of cancer multi-omics analysis revealed the oncogenic pathway can show important role through cancer types using omics approach. Cancer mutations, copy-number alterations, mRNA expression, gene fusions and DNA methylation data of breast cancer 1,108 tumors profiled sample is available in The Cancer Genome Atlas (TCGA). We analysed the mechanisms and patterns of somatic alterations in 10 oncogenic pathways. Also identified the landscape of pathway alterations in breast cancer with stratified into subtypes and patterns of co-occurrence by integration of clinical samples. Identified pathways signatures associated with 313 driver genes used to analysis anticancer drug response of individuals by integrating the multi-omics data of breast cancer. Further, pathway based signatures analyse using anticancer drug response with different clinical outcomes will assist in designing better prognostic or predictive biomarkers.

**Keywords:** Multi-omics, oncogenic pathways, Breast cancer, Cancer driver genes, TCGA

**In-vitro phytochemical screening of leaf extracts of *Nyctanthes arbor-tristis* L. for potential bioactive compounds**

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**Abstract:** *Nyctanthes arbor-tristis* L. is a medicinally important plant in the folklore and herbal therapy. The leaves of *Nyctanthes arbor-tristis* L. have been used in ancient Ayurveda. The present study focus on two extracts obtained from the leaves of *Nyctanthes arbor-tristis* L. viz. aqueous extract and ethanolic extract. The qualitative and quantitative analysis was done for quantification. The characterization of the phytochemical extracts was carried out using FTIR and the results shows presence of many functional groups reflecting the results obtained during qualitative analysis. Further, LCMS analysis was performed to characterize the chemical constituents in the extracts that revealed many biologically important compounds.

*Anti-microbial assays were carried out for each extract for six bacteria. Both extracts show antibacterial activity against all bacteria except S. aureus. DPPH free radical scavenging assay was performed to assess the potential anti-oxidant capacity of the extracts. Both the extracts were observed to show powerful anti-oxidant activity which, might be attributed to presence of phenolics, flavonoids, tannins*

**Keywords:** *Nyctanthes arbor-tristis* L, FTIR, LCMS, antimicrobial assay, DPPH assay, aqueous extracts, ethanolic extracts

### **Design and development of health care robot.**

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**Abstract:** The pandemic situation has brutally affected the health care sector of each country. Every country tried their best to come up with new methodologies and techniques to control the situation. Considering the situation of health care statistics of India, the robot is a must to maintain the preventive measures with which the pandemic situation can improve a lot. The main aim of the proposed work is to design and develop an autonomous robot that will help us to follow all the rules which are required to create a healthy environment. The proposed model design is user-friendly, cost-effective, and multifunctional. The proposed model will help the health care sector to prevent from the diseases by automatic sanitization, checking the oxygen pulse and body temperature. Further with the navigation system, it will able to plan its path and with the help of a vision system, it will give instructions to wear a mask and to keep social distancing. The proposed robotic system can be used in the crowded places such as hospitals, colleges, schools, railway stations, airports, etc to serve the people for their safety.

**Keywords:** Autonomous robots, Modern technology, Healthcare sector.

## **Biological Toxicity analysis of Biopolymeric Silver Nano Drug Delivery System**

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**Abstract:** This present work was aimed to discuss the potential of Pullulan-mediated Silver-Curcumin nanoconjugate (AgNPs) for its in-vivo safety through biological toxicity analysis. The biological toxicity evaluation comprises two major analyses viz. Acute Dermal Toxicity Study (ADT), Repeated Dose Dermal Toxicity study (RDT). Pullulan mediated silver-curcumin nanoconjugate was synthesized using chemical substrate method taking AgNO<sub>3</sub> as precursor molecule. The data clearly shows that the nanoconjugate tested at 2000 mg/kg, dosage routine didn't elicit mortality in test animals. The median lethal dose (LD50) of the conjugate after dermal route as a single application in rats was estimated to be more than 2000 mg/kg b.w. making it Category 5 entity, as per the defined OECD guidelines for chemicals classification. Thus the study provides primary data showing the potential of this nanoconjugate as successful candidate for nano conjugated drug delivery system.

**Keywords:** Nano-drug delivery, nanoparticle, biopolymer.

## **Computational and Docking Studies of Chromone Derivatives as Selective Src Family Tyrosine Kinase Inhibitors**

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**Abstract:** Src family kinases (SFKs) are a family of tyrosine kinases which play a critical role in signal transduction. *In-silico* studies such as virtual screening and molecular modeling have proven to be useful in developing kinase inhibitors. A library of chromone compounds was synthesized and was prioritized to obtain a lead chromone compound (MMK014) with desired in-silico properties. Docking study was performed to analyze the binding mode of MMK014 chromone compound against 8 target SFK proteins. The best interaction was obtained for Yes protein (-7.61 kcal/mol) and cSrc protein (-6.5 kcal/mol). Further molecular dynamics and simulation based study revealed that MMK014 compound showed selectivity for leucine, valine, lysine and aspartate residues. It is envisaged that the molecular modeling studies will help us in developing a better anti-SFK drug in near future.

## Spice Drug Potential for Arthritis using Ayurvedic & pharmacokinetic methods

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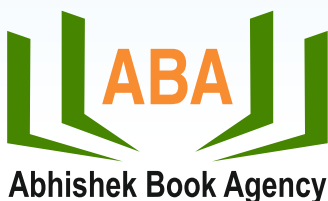
**Abstract:** Arthritis is commonly emergic ailment of the elderly globally and a major health burden. There is no safe or highly effective modern medicine to treat it yet though Non steroidal anti inflammaotory drug (NSAID) therapy is common despite many adverse drug reactions (ADR) such as stomach upset. Consuming gums of Guggulu (*Commiphora wightii*) i.e. Indian Bdellium/ Myrrh & Frankinsense (*Boswellia serrata*) still are top herbal cures but threatened with extinction by overharvest. Hence, spices also used traditionally in Aarthritis are explored for sustainability. Docking study was performed on the key bioactive compounds important spices w.r.t. COX2 active site (PDB ID 51kR obtained from PDBsum). Molecule with having the maximum stability and lowest binding energy is '10-Gingerol' from Ginger (-7.34 kcal/ mol), followed by '8-Shagalol' (-7.51) also from Ginger, Both values are lower than methotrexate (-8.6), the standard NSAID used widely and synthetically designed 'best' molecule- i.e. 4-(4-methyl-1-piperaziny)-2-phenyl[1]benzofuro[3,2-d]pyrimidine found by Saudi Arabian researchers. Three other spice ingredients have closeby values viz. 'Curcumin' (Turmeric, -8.66), 'Apigenin' (Coriander, -9.63), and Piperine (Black Pepper, -9.99). Diosgenin from Fenugreek had the lowset value (-6.8) but outside the active s ite so not feasible. Ginger and Turmeric are considered of "hot" nature in Ayurveda and cause bleeding if consumed in excess, and administred with Milk or Ghee (, considered a coolent and improves their bioavailability due to fatty nature. Synergistic effect of the spice combination of these spices are now being studied for drug design.

**Keywords:** Arthritis, anti-inflammatory, spices, Ginger, docking, Ayurveda, bioactive





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