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February 27-29, 2020

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(ICSS-2020)

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Prof. Manju Bansal, Indian Institute of Science, Bengaluru

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Prof. Renaud Jolivet, University of Geneva, Switzerland

The brain's heterocellular complexity through the lens of brain energetics **Dr. Jeyanthy Eswaran,** Newcastle University of Medicine Malaysia

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Decoding epigenetic circuitry in diseases – an interdisciplinary approach Lunch

Poster Session I

Prof. Palani Balaya, National University of Singapore

Can We Design Safe Large Scale Energy Storage Systems?

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Electrochemical Energy Storage Systems: Great Challenges and Opportunities

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How prebiotic selection pressures shape the evolution of protocells

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Customized Functional Organic Nanomaterials for Catalysis, Drug Delivery and Optoelectronic Applications

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13.30-14.15	**SASTRA - C.N.R. Rao Award Lecture II** **Prof. S. Sampath**, Indian Institute of Science, Bengaluru *Interfacial Electrochemical Studies: Use of Nanostructured- Surfaces and Catalysts*
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Invited Lectures

IL-01

Role of DNA Structural Variability in Promoter Function: A Composite Study using Physics, Chemistry & Biology

Prof. Manju Bansal

Molecular Biophysics Unit, Indian Institute of Science, Bangalore Email: mb@iisc.ac.in

Structural stability and flexibility both play important roles in efficient functioning of biological macromolecules such as proteins and nucleic acids. The talk will outline the basic principles that determine these properties and some of our recent work wherein structural variability or flexibility in DNA is found to be strongly correlated with its function. Experimental and *in silico* analyses of promoter regions of genomic DNA indicate that while there is considerable variation in their base composition and sequence, leading to possible occurrence of even non-B-DNA structural motifs, some DNA structural properties show significant conservation. We have analyzed various structural features, such as stability, bendability, intrinsic curvature and groove width, in promoter regions of both prokaryotic and eukaryotic genomes and compared these with coding regions. Published experimental data from transcriptome analysis, correlates well with these DNA structural features.

We have also performed high-throughput *in vitro* and *in silico* analyses to understand the influence of flanking sequences outside the cognate sites in binding of three most prevalent Transcription Factors (TFs) – belonging to Zinc finger, homeodomain, and bZIP families. It is found that local structural features of sequences flanking the consensus motifs are also instrumental in determining the binding affinity of TFs. DNA structural models employed in our study use principles of physics, chemistry and statistical analysis to provide mechanistic insights into DNA-protein recognition, which can help refine bioinformatics tools for improved binding site search prediction and modelling of TF binding.

Acknowledgement:

V. Rajesh Yella, Debostuti Ghoshdastidar, Indian Institute of Science, Bangalore 560012, India & Devesh Bhimsaria, Aseem Z. Ansari, University of Wisconsin-Madison, Madison, USA.

IL-02

The brain's heterocellular complexity through the lens of brain energetics

Prof. Renaud Jolivet

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The brain consumes an inordinate amount of energy with respect to its size, and consists of an intricate network of neurones, vasculature and glial cells. I will discuss how energetic considerations can be combined to information theory to ask questions about how the brain balances the competing needs to save energy, while retaining reasonable performance. In particular, I will show how energetic considerations and information theory can be combined to explain certain synaptic features. I will then discuss how these ideas can be expanded to the network level. Finally, I will discuss how brain energetics and information theory can be combined to develop a computational framework for the brain's heterocellular circuits.

IL-03

Genomic Medicine and Emerging Technologies

Dr. Jeyanthy Eswaran

Research lead and Asst Dean of Research
Newcastle University Medicine Malaysia, Newcastle University, UK, Johor, Malaysia Email: Jeyanthy.Eswaran@newcastle.edu.my

The evolution of genomic technologies open unprecedented opportunities to understand the role of genetics in human diseases on a global scale and enable the development of personalised medicine. A number of countries have begun to integrate genomic medicine into their health care system. This represents breaking boundaries in clinical medicine from 'one-size-fits-all' approach to tailored care and targeted therapies for patients suffering from various disorders including cancers. This talk will provide a comprehensive overview of how the multi disciplinary, trans national research plays a central role in the development of precision cancer medicine. Moreover, the current state of personalized medicine in cancer and the challenges involved in the broad implementation of genomics in clinical practice and improving health service delivery will also be discussed.

IL-04

Decoding epigenetic circuitry in diseases – an interdisciplinary approach

Dr. M. Vijayalakshmi

Institute of Bioinformatics and Applied Biotechnology (IBAB), Bangalore Email: mviji@ibab.ac.in

Alterations in epigenetic modifications and chromatin structure are known to drive tumour initiation and progression. The clinical importance of p53 mutations in colon cancer emphasises the need to understand the interplay between p53 signalling and epigenetic regulation in colon cancer. This talk would detail our pursuit to understanding epigenetic modulation in colon cancer through imaging, biochemical and genomic approached to understand the influence of these alterations in the 3D organisation of the genome and our preliminary attempts to understand genome wide changes in neuropsychiatric disorders.

IL-05

Can We Design Safe Large Scale Energy Storage Systems?

Dr. Palani Balaya

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The escalating trend of mitigating greenhouse gas emissions by replacing fossil fuel energy with renewable energy has increased the demand for large-scale energy storage systems (ESS). Lithium-ion batteries (LIBs) have proven to be one of the best options for such stationary storage applications. However, LIB technology has its own concerns over cost and safety. Lithium consumption has increased significantly in last three decades mainly due to the rapid growth of LIB markets for mobile and grid storage applications. On the other hand, fire safety is another important factor in large-scale ESS as LIBs, in general, are likely to experience thermal runaway in harsh or abusive environments. To overcome such concerns, Na-ion battery (NIB) is proclaimed to be - one of the best candidates to substitute LIB, where the footprint and weight of the battery are not the major concerns.

In this talk, a comprehensive study on electrolyte, anode and cathode for an industry-standard non-flammable NIB will be presented. More specifically, investigations on thermal stability and related solid-electrolyte interphase (SEI) studies on hard carbon (HC) anode material, and two types of cathode, modified $Na_3V_2(PO_4)_3$ (NVP) and O3-type layered oxide will be discussed. We will also present performance of 18650-type commercial cells fabricated using modified NVP as cathode with HC as anode. Heat generation and associated internal resistances of such 18650 type cells will also be discussed.

IL-06

Electrochemical Energy Storage Systems: Great Challenges and Opportunities

Dr. P. Ragupathy

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As world population and economic prosperity increase simultaneously along with substantial change in human life style, the total energy consumption increases to large extent. The present annual global energy consumption is found to be ~ 15 TW (terawatts) and more than 80% of this requirement is met from non-renewable sources such as oil, coal and gas. By 2050, the energy demand is expected to reach 30 TW. Traditional non-renewable resources have a limited stock and their use for electricity production poses severe environmental issues such as CO_2 emission and hence global warming. In such a scenario, generation of clean energy to meet the future energy demand is the need of interest and much discussed topic at government and scientific levels. This becomes essential to sustain the social and economic development achieved during the past decades.

In spite of huge amount of energy generated by renewable sources, they have their own limitations such as unpredictable and inconsistent power supply. The impact of renewable energies will not be fully realized, unless an efficient route is found to store the energy generated by renewable energies. In this perspective, electrochemical energy systems (EESs) are promising alternative energy sources owing to their direct energy conversion without intermediate step, high efficiency of conversion, absence of moving parts and hence minimum noise level, minimum pollution, portability, miniaturization and convenience to scale up. Here, EES plays an important role as storage devices to storage the energy which can be utilized wherever and whenever it is needed. Particularly, advanced/novel materials hold the key for future development of clean energy generation and storage due to their unique physical and chemical properties offer unprecedented opportunities in energy technology. Thus, the present talk will focus an overview of ***'Electrochemical Energy Storage Systems: Great Challenges and Opportunities'***.

IL-07

How prebiotic selection pressures shape the evolution of protocells

Dr. Rajamani Sudha

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Abstract: Protocells are primitive cellular entities that are thought to have emerged during the dawn of life on Earth. Their membranes are thought to be made up of mixtures of single chain amphiphiles, such as fatty acids and their derivatives; moieties that would have been part of the complex prebiotic chemical landscape. In addition to their composition, the physico-chemical properties of these prebiological membranes would have been significantly affected and regulated by the physical environment that they were present in. In this talk, I will discuss what we have gleaned from studying the properties of prebiotically relevant membrane systems under pertinent selection pressures such as stability under varying pH, divalent ion concentrations etc. Our results demonstrate how environmental constraints would have acted as important selection pressures to shape the evolution of prebiological membranes. Our results also illustrate that hetergeneous membrane systems are more stable and robust to multiple selection pressures, thereby making them more suitable for supporting protocellular life.

IL-08

Customized Functional Organic Nanomaterials for Catalysis, Drug Delivery and Optoelectronic Applications

Dr. Govindasamy Jayamurugan

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We use synthetic chemistry as a tool to develop rationally designed systems for specific problems faced in the area of catalysis, drug delivery and optoelectronic applications. Our lab is actively working on the utilization of carbohydrates available abundantly as bio mass, and converting it in to the functionalized carbohydrates using chemo-processing as a tool. The target was achieved by the combination of nanotechnology and synthetic modifications. My talk will comprise of three area (Biology, Chemistry, and Physical) as the theme of this conference covers interdisciplinary sciences.

The first part deals with the long standing problem faced in cancer therapy i.e. the selective killing of cancer cells and biocompatibility of the drug and nanocarrier. To contribute in this, we have developed a nanocarrier which is capable of selective killing of colorectal cancer cells via synthetic lethality approach with high biocompatibility due to functional tri-layer polymeric system.[1] In an another study, we took a problem to demonstrate which type of nanocarrier for pesticide delivery would be viable among organic and/or hybrid nanoparticles.[2] Our study answers for the question, which is the viable method for better encapsulation and sustained release among the various functionalized and unfunctionalized polysaccharides? Further, we demonstrate that subsequent modifications and anchoring appropriate metal-nanoparticles provided a very active, recoverable catalyst for the selective organic transformation reactions under greener conditions.[3a] This green catalyst was successfully used for the production of anti-epileptic drug in an industrial friendly method.[3b]

The 3rd part deals with the development of novel class of optoelectronic materials. Last decade has witnessed a tremendous interest in donor substituted poly-cyano olefins based push -pull chromophores in order to miniaturize the electronic world, owing to its click type synthesis, high intramolecular charge-transfer, redox behavior and with high thermal stability. In this work, we demonstrate that urea-functionalized 4-ethynylbenzenes undergo facile formal [2+2] cycloaddition followed by retroelectrocyclization upon reaction with tetracyanoethylene to provide 1,1,4,4-tetracyanobuta-1,3-dienes based push-pull chromophores. Unlike *N,N'*-dialkylamino group, urea functionalization offers easy access to further functionalization on these chromophores and exhibits remarkable white light emission property apart from the inherent properties like intramolecular charge-transfer band and redox behavior.[4] Currently, we are exploring nanoparticles system capped with this novel chromophores for various applications like solar cells, sensing, photodynamic therapy and bio-imaging applications.

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IL-09 **SASTRA-G. N. Ramachandran Award Lecture**

Structural basis of the exploitation of innate immunity proteins as new generation antibiotics

Prof. T. P. Singh
Department of Biophysics, All India Institute of Medical Sciences, New Delhi - 110029
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Considering the alarming rise in the incidence of bacterial resistance to currently known antibiotics, there is a desperate need to develop bacterial resistance-free new antibiotics. There have been many efforts to design new antibacterial agents using natural products, combinatorial chemistry approaches, structure based design and other development approaches of synthetic compound libraries. In order to overcome the problem of antibiotic resistance, the available antibiotics need to be modified accordingly as well new approaches of drug discovery must also be pursued vigorously.

We have been working on an entirely new concept of introducing the innate immune proteins as protein antibiotics by exploiting the differences in the potencies of innate immune proteins from different animal species. It has been well known that the proteins of the innate immune system provide the first line of defense against infecting microbes. These proteins recognize the conserved motifs that are present on the cell walls of bacteria. Thus the success of the innate immune system depends on the affinity of these proteins towards the bacterial cell wall molecules. The conserved motifs of microbial cell walls are called pathogen associated molecular patterns (PAMPs) that include the well-known peptidoglycans (PGN) and lipopolysaccharides (LPS) of Gram-negative bacteria, PGN and lipoteichoic acid (LTA) of the Gram-positive bacteria and mycolic acid (MA) and other fatty acids of *Mycobacterium tuberculosis*. These PAMPs are classified into two groups: (i) those which contain glycan moieties such PGN, LPS, LTA etc. and (ii) those that are derivatives of fatty acids such as MA. Therefore, there should be two independent binding sites for the two different types of PAMPs. The PAMPs are specifically recognized by innate immunity molecules which are historically known as peptidoglycan recognition proteins (PGRPs).The epidemiological data have shown that the extremophiles such as camels, yak and porcine have the lowest rates of infections. We have determined the structures of PGRP-S from camel, yak and porcine. The structures revealed that the PGRP-S from camel and yak form two functional dimers whereas the human protein acts as a monomer. As a result of dimerization, a deep binding cleft is formed in the camel and yak proteins whereas only a shallow cleft is present in the case of human monomeric protein. Because of this, the potencies of camel and yak proteins are much higher than the same protein from other species including human, bovine, horse, goat and sheep. Thus, if camel/yak protein is used or a suitably modified human protein is prepared and used, the fight against bacterial infections will improve considerably.

The mechanism of action of PGRP-S involves an effective sequestration of bacteria which eventually leads to the killing of bacteria. Since PGRP-S interacts with bacterial cell wall molecules, the kinetics of bacterial cell death appears to be similar to those of antibiotics which inhibit the biosynthesis of PGN. Due to this similarity, PGRP -S protein from innate immune system is termed as “protein antibiotic” and since it binds to different bacterial cell wall molecules, the issues of side effects and resistance will not arise and since the potency is much higher, the invading bacteria can be tackled rapidly by using such an innate immune protein as a therapeutic molecule.

IL-10 **SASTRA - Obaid Siddiqi Award Lecture**

Understanding the sources of regenerative capacities in animals

Prof. Alejandro Sánchez Alvarado

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Plurtipotent stem cells are generally associated with embryonic stages of animal development. In mice, for example, embryonic stem cells normally exist for a few hours after which they are no longer maintained in the embryo. The quality of these stem cells determines the fitness of the resulting progeny and tissues, including the germline, which ultimately will determine the survival and perpetuation of the species. As such, when we think about natural selection, we conceive of this process operating at the level of either individuals or communities of individuals. In some organisms, however, it is normal for pluri- if not totipotent cells to persist beyond embryogenesis and carry out both tissue homeostatic and regenerative functions in the adult. The persistence of pluripotent stem cells beyond embryogenesis is a common feature of plants but it is also known to occur in many animal species. One such group of animal are planarians, members of the phylum Platyhelminthes, which are known to possess abundant numbers of adult pluripotent stem cells known as neoblasts. Unlike most other cells in animal body plans, stem cells self-renew, form clones and perpetuate themselves throughout the life of the animal. In planarians, which can reproduce asexually, these pluripotent stem cells perpetuate themselves across generations as well. Hence, competition among these pluripotent cell clones is likely to be constant, essentially transforming neoblasts into units of natural selection. Of the thousands of species known thus far, the planarian *Schmidtea mediterranea* has become a fruitful research organism in which to explore and dissect the functions, behaviors and properties of these adult pluripotent stem cells. Their embryonic origin, diversity in adults, prospective isolation and variable genomic output will be discussed in the context of both tissue homeostasis and regeneration.

IL-11 **SASTRA - Obaid Siddiqi Award Lecture**

Molecules, memory, and mathematical models

Prof. Upinder S. Bhalla

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Molecular events underlie all cellular processes, including memory. The strength of connections between neurons (synapses) is an important locus of memory storage, and there are several ideas about how molecular events in synapses could translate into changes in connection strengths. This picture is complicated by two peculiarities of molecular events at synaptic scales: signal flow is very noisy, and the molecules themselves turn over rapidly. This poses a conceptual problem: how does one store information reliably when the substrate for storage is noisy and short-lived? I will explore how one crosses scales of brain function to relate classical conditioning to molecular events. Then I will consider how these molecular events might overcome the two problems of noise and molecular turnover. This analysis relies on the use of mathematical concepts of bistability, and extensive computer simulation. Finally, I will step back again to examine what we know of how more complex memories may also arise from the action of molecules in synapses on cells in networks.

IL-12 **SASTRA – C.N.R. Rao Award Lecture**

From Molecules to Functional Materials: Amorphous OLEDs and Crystalline MOFs

Prof. Jarugu Narasimha Moorthy

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The properties of bulk organic materials are determined by organization of their constituents molecules. Implicit in it is the fact that the structures of organic molecules that make up the bulk materials crucially control the properties of the latter. We believe in the fact that 'organic structure is quintessential to control both reactivity as well as molecular organization, and hence the properties of materials'.

I will exemplify how organic compounds may be engineered in a bottom-up fashion by a diligent design to develop two distinct classes of materials, namely, amorphous organic light emitting diodes[1] and ordered porous metal-organic materials.[2] As to the latter in particular, I will present our very recent de novo approaches to the development of stimuli-responsive 2D metal-organic nanosheets (MONs).[3]

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IL-13 **SASTRA – C.N.R. Rao Award Lecture**

Interfacial Electrochemical Studies: Use of Nanostructured- Surfaces and Catalysts

Prof. S. Sampath

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Electrochemistry, an interfacial science where redox reactions occur at electrode / electrolyte interfaces, has been in the forefront of research, particularly on modified surfaces and new materials. There have been intense efforts directed towards finding efficient electrocatalysts for various reactions of interest. The present lecture will describe some of our work carried out to understand the fundamental aspects involved in electrocatalysis related to energy storage systems and other aspects.

IL-14

Nurturing of biology by Chemistry and Physics

Prof. Pinak Chakrabarti

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There is cross-talk between all the branches of science. Coming from an institute founded by Sir JC Bose, who is considered to be the first biophysicist in the world, it is awe-inspiring to realize the instrumentations that he had fabricated to quantify and study plants. Like a river originating in mountains, flowing through the plains before merging into the sea, all the spectroscopic techniques were developed in physics labs, applied to understand the chemical world and eventually the life processes. One of the important tools the structural biologists use is the Ramachandran plot, which was derived using the non-bonded contact distances as seen in small molecule crystal structure. Protein structures were thus understood using chemistry data. The Nobel Prize in Chemistry 2008 was awarded to scientists working on green fluorescent protein (GFP). A glowing protein discovered in jellyfish has been used as a probe to view and understand the inner workings of cells. Nanoparticles developed in physics labs have been used as biosensors and drug-delivery vehicles. "All biology is computational biology" (Markowetz, PLoS Biology (2017). Taxonomy, evolution at the heart of biology are getting a new perspective based on theoretical analyses of large databases. A new field, bioinformatics that draws heavily from mathematics, statistics, data mining, computer algorithm, is revolutionizing drug development and experimental designs. There are cross-talks between different branches of life sciences also. The concept of miRNA was developed from observations in plant sciences.

IL-15

Binding affinity of protein- protein complexes: structural analysis, discrimination, prediction and mutational effects

Prof. M. Michael Gromiha

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Protein-protein interactions play crucial roles in many biological processes and responsible for smooth functioning of the machinery in living organisms. Predicting the binding affinity of protein-protein complexes and understanding the recognition mechanism are challenging problems in computational and molecular biology (1,2). Using a generalized energy based approach we showed that charged and aromatic residues are important for binding in protein-protein complexes. These residues influence to form cation–p, electrostatic and aromatic interactions. Our observations have been verified with the experimental binding specificity of protein-protein complexes and found good agreement with experiments (3). Further, we have developed algorithms for discriminating protein-protein complexes based on their binding affinities (4), predicting the binding affinity (5) and constructing protein-protein interaction networks (6). We have also analyzed the integrative role of amino acid residues involved in both stability and binding (7). Recently, we developed a database for binding affinity of protein-protein complexes and their mutants (8). Utilizing the database, we analyzed the factors influencing the affinity of single mutants and the additivity effects of double mutants (9). The salient features of the results will be discussed.

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IL-16

Spontaneous conformational transitions of A…A mismatch in d(CAA.TAG) provide a clue for the interaction with mismatch repair proteins

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Base pair mismatches can erroneously be incorporated in the DNA during replication and recombination *etc*. Here, the influence of A…A mismatch in d(CAA.TAG) is explored using molecular dynamics (MD) simulation, umbrella sampling simulation, circular dichroism (CD) and NMR techniques. The MD simulations reveal that A…A mismatch experiences a variety of spontaneous events such as base flipping, base extrusion, *etc.*, facilitating B-Z junction formation. A…A mismatch may assume such conformational transitions to circumvent the effect of nonisostericity with the flanking canonical base pairs so as to get accommodated in the DNA. CD and 1D proton NMR experiments further reveal that the extent of B-Z junction increases when the number of A…A mismatch in $d(CAA.TAG)_{n=1\text{-}to\text{-}5}$ increases. The umbrella sampling simulation indicates that the mismatch samples *anti…+syn/+syn…anti, anti…anti & +syn…+syn glycosyl* conformations concomitant with a variety of hydrogen bonding patterns and minor or major groove extrahelical movements. These transitions frequently happen in *anti…anti* region compared to the other three regions as revealed from the lifetime of these states. Further, 2D-NOESY experiments indicate that the number of cross-peaks diminish with the increasing number of A…A mismatch implying its dynamic nature. Such a spontaneous extrahelical movement in A…A mismatch may be a key pre-trapping event in the mismatch repair as it drives the bases accessible to the sophisticated repair proteins.

IL-17

Insulin action and oxidative stress in type 2 diabetes

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Type 2 diabetes mellitus (T2DM) is typically an age-onset disease with several underlying factors that eventually result in hyperglycemia. Although a lot is known about the disease, both clinically and biologically, the management of glucose remains the key objective of treatment in T2DM. In my talk I will describe not only mathematical models but also some clinical studies in which we have attempted to enlarge the scope of diabetes management beyond glucose, to include aspects of insulin action as well oxidative stress. This is joint work going back nearly a decade with Prof. S. Ghaskadbi, Pune University, and more recently Dr. U. Divate at Jehangir Hospital, Pune, and others.

IL-18

India-based Neutrino Observatory: Present Status and Physics Goals

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Neutrinos play critically important roles in several important fields of physics including elementary-particle physics, nuclear physics, nuclear and parti- cle astrophysics, and cosmology. Compared to the other fermions, the elusive na- ture of the neutrinos has made them extremely difficult to study in detail. In spite of the challenges, neutrino physics has progressed dramatically over the past two decades, propelled by the surprising discoveries that neutrinos have mass and that they change their flavor as they move in space and time. Marvellous data from world- class experiments involving neutrinos from the Sun's core, the Earth's atmosphere, nuclear reactors, and accelerators have firmly established a phenomena known as 'neutrino mass-induced flavor oscillation', which suggests that neutrinos have mass and they mix with each other, providing an exclusive evidence for physics beyond the Standard Model. Such a landmark discovery of fundamental significance, re- cently awarded with the Nobel Prize, sets a fantastic example of a roadmap in which both theoretical understanding and experimental achievements have walked hand in hand to uncover a new landscape in neutrino physics, with a promising future for continued discovery. I will shed light on these interesting developments in neu- trino physics during the first half of my talk. To carry out research in the emerging field of neutrino physics, the India-based Neutrino Observatory (INO) Collaboration is making sincere attempts to build a world-class underground laboratory at Pottipu- ram in Bodi West hills of Theni District of Tamil Nadu. Once completed, it will be the largest basic science project in India. The proposed laboratory will house a 50 kilo- ton magnetized iron calorimeter (ICAL) detector to study the atmospheric neutrinos and antineutrinos separately over a wide range of energies and path lengths. This ambitious INO project has already drawn the worldwide attention of international scientists. During the second half of my talk, I will also discuss about the present sta- tus and physics reach of the INO project, which is one of the flagship mega-science projects of our country.

IL-19

Data-driven discoveries in chemical compound space: Trends and Challenges

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The MolDis repository (https://moldis.tifrh.res.in/index.html) under development at TIFR Hyderabad aims to provide a publicly accessible analytics platform for Big Data of computed molecular/materials properties. Presently massively large datasets are being generated for a multitude of domains of application. The talk will give an overview of the MolDis initiative and discuss the critical role machine-learning algorithms play in this project. Global trends in the emerging area of data-driven computational chemistry/materials science will be discussed along with comments on problems that remain open as yet.

IL-20

Computational Analysis of Dynamics-Function Relationship in Mammalian Lipases

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Enzymes are catalysts of biochemical reactions in living organisms. Lipases are vital digestive enzymes that hydrolyse triglycerides into free fatty acids. The activity of pancreatic lipases is controlled by a lid covering the active site and a coenzyme known as colipase. In the active state, the lid remains in its open conformation stabilized by the binding of coenzyme. In the absence of substrate and coenzyme, the lid attains a closed conformation in water; however, polar-organic solvents can induce the lid to attain its open conformation which has an industrial relevance. These sub-microsecond transitions are investigated by molecular dynamics simulation to understand the residue-level conformational changes, dihedral constrains and intra-domain interactions during these processes. Further, a structural model is developed by computational methods to address the essentiality of the presence of substrate molecules at micellar-concentration to induce the activity of pancreatic lipase. The model also explains the role of the dynamics of colipase on the protein's activity particularly at interfacial surfaces.

Oral Presentations

O-01

Influence of terminal group on the structural, thermal and hydration properties of gold-fullerene nanocomposite

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We have investigated the influence of the methyl (hydrophobic) and hydroxy (hydrophilic) terminal groups on the structural, thermal and hydration properties of gold-fullerene nanocomposite using molecular dynamics simulation technique. The van der Waals interactions between the thiol capped gold nanoparticle and fullerene have driven the formation of gold-fullerene nanocomposite. The active ter-minal methyl and hydroxy groups have influ-enced the time of formation of self-assembly, stability, conformation and dynamics of the thiol chains, specific heat capacity and hydration properties of the gold-fullerene nanocomposite. The value of the specific heat capacity of the hydroxy gold-fullerene nanocomposite is found to be higher than the methyl gold-fullerene nanocomposite. The variation observed in the specific heat capacity of the gold-fuller-ene nanocomposite may be attributed to the factors like molecular weight, conformation of the thiol chains which can vary the fre-quency of oscillation.

The hydration properties of the gold-fullerene nanocomposite such as structure of hydration layer, population of interfacial water molecules, hydrogen bonds, orientation of water molecules, water residence time and solvent accessible surface area have been estimated. The hydroxy gold-fullerene nanocomposite was found to have higher wettability than the methyl gold-fullerene nanocomposite. The results of this simulation study, may aid the understanding and development of novel gold-fullerene nanostructures for modulating their structural, thermal and hydration properties through the modification of their surface functional groups.

O-02

Transparent and smart electrochromic supercapacitors with networked electrodes

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Transparent and flexible energy storage devices have received immense attention due to their suitability for innovative electronics and displays. However, it remains a great challenge to fabricate devices with high storage capacity and high degree of transmittance. This study describes a simple process for fabrication of supercapacitors with ≈75% of visible transparency and areal capacitance of ≈3 mF cm−2 with high stability tested over 5000 cycles of charging and discharging. The electrodes consist of Au wire networks obtained by a simple crackle template method which are coated with MnO2 nanostructures by electrodeposition process. Importantly, the membrane separator itself is employed as substrate to bring in the desired transparency and light weight while additionally exploiting its po-rous nature in enhancing the interaction of electrolyte with the active material from both sides of the substrate, thereby enhancing the storage capacity.1 The method opens up new ways for fabricating transparent devices. Furthermore, smart electrochromic supercapacitors are fabricated using Au mesh and polyaniline (PANI) electrodes. What is attractive about this device is that it can switch its color rapidly, yellow, green, or blue, depending on

the operable voltage window that should serve to indicate the level of energy stored in the su-percapacitor, visually.2

O-03

Investigating the role of N-glycan in the interaction of biomarker human myelin oligodendrocyte glycoprotein with the human leukocyte antigen

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Myelin is a multi-laminar lipid sheath that surrounds nerve cells and acts as an insulating layer to increase the speed of stimuli being transmitted between nerves. The myelin oligodendrocyte glycoprotein (MOG) is found in the outer layer of the myelin sheath. This protein under certain physiological conditions acts as an auto-antigen. This leads to the da-mage of the myelin sheath called demyelina-tion. MOG has a single N-glycosylation site at the residue N31 and the effect of glycosylation in the process of demyelination is not under-stood to date. The mechanism of MOG reco-gnized by human leukocyte antigen (HLA)/TCR is not yet studied.

In this computational study, we focused on identifying the key residues in human MOG which interact with HLA. As the previous studies showed the significant role of N-glycan in the conformation changes of MOG interac-ting with (8-18C5) Fab antibodies, the glycosylation effect in the interacting key MOG residues was studied. Both the monomer and dimer of human MOG were homology modelled and the HLA was taken from the existing PDB (1YMM). The protein MOG and HLA were docked using the Cluspro program. Four systems consisting of monomer MOG -HLA, dimer MOG-HLA and their presence in N-glycan were considered for the study. Each system was solvated using TIP3P water molecules and counterions were added. The systems were minimized using the conjugate gradient method with the amberff14SB force field in the AMBER18 program. The well-mi-nimized systems were equilibrated for 5ns in the NPT ensemble and further subjected to molecular dynamics simulation for 50ns. Coordinates and energies were recorded at every 10ps which yielded 5000 conformations.

The main results show that the N-glycan has a significant role in identifying the key residues of MOG that interact with HLA.

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O-04

MYC dependent regulation of SWI/SNF chromatin remodelling complex

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Precise positioning of nucleosomes at the gene regulatory elements mediated by the SWI/SNF family of remodelling complex is important for the transcriptional regulation of genes. A wide set of genes are either positively or negatively regulated by SWI/SNF. In higher eukaryotes, around thirty genes were found to code for SWI/SNF subunits. The con-struction of a gene regulatory network of SWI/SNF subunits identifies MYC as a common regulator for many of the SWI/SNF subunit genes. A meta-analysis study was conducted to investigate the MYC dependent

regulation of SWI/SNF remodelling complex. Subunit information and the promoter sequences of the subunit genes were used to find the canonical E-box motif and its variants. Detailed analysis of mouse and human ChIP-Seq at the SWI/SNF subunit loci indicates the presence of MYC binding peaks overlapping with E-boxes. The co-expression correlation and the differential expression analysis of wt vs. MYC perturbed MEFs indicate the MYC dependent regulation of some of the SWI/SNF subunits. The extension of the analysis was done on MYC proficient and MYC deficient embryonic fibroblast cell lines, TGR1 and HO15, and in one of the MYC amplified can-cer types, Medulloblastoma. A transcriptional regulatory feedback loop between MYC and SWI/SNF could be a major factor contributing to the aggressiveness of MYC dependent can-cers.

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O-05

Exploring the competence of plant derivatives to control bacterial leaf blight disease in rice-an *in-silico* approach

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Rice is the most important staple food for almost half of the world's population. *Xanthomonas oryzae* pv. *oryzae* (Xoo), strain Pxo99A causes Bacterial leaf blight in rice and it leads to 50% of yield loss. Hence it is more significant to control the disease in order to prevent the yield loss. Currently various agrochemicals are used to control the disease which in turn is found to have various adverse effects on environment and human health. In the present study the anti-bacterial activity of plant derivatives from different plants has been examined through systematic *in silico* investigation. The results revealed that the plant derivatives were found to exhibit better anti-bacterial activity than that of commercially available agrochemicals. Therefore, it could be suggested that the natural compounds extracted from plant sources can be used as an alternative to agrochemicals in controlling the rice bacterial blight. These compounds would provide a cost effective and eco-friendly means to control the disease and increase the crop yield.

O-06

A new ambuic acid derivatives anticancer secondary metabolites from marine algae endophytic fungi and their structural elucidation molecular mechanism underlaying anticancer effects

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The new ambuic acid derivatives anticancer compound was isolated from the marine algae endophytic fungi. The structure of the compounds was elucidated on the basis of comprehensive spectral analysis (UV, IR, 1H, 13C- as well as HRESI–MS). Further the compound evaluated the cytotoxicity effect on the human cervical cell line (HeLa) and Breast cancer cell line (MCF-7) The results obtained from the MTT assay showed that new ambuic acid significantly inhibited cytotoxicity against MCF-7 cell line. The lowest IC_{50} of 27.01± μM is obtained in MCF-7; therefore, all investigations regarding the antiproliferative properties of new ambuic acid derivatives

compound were carried out on the MCf-7 cell line. The new ambuic acid induced changes characteristic of apoptosis such as chromatin condensation, cell shrinkage and formation of apoptotic bodies in new ambuic acid derivati-ves compound treated cells. The new ambuic acid treatment triggers the mitochondria-mediated apoptosis and cell cycle G1 phase arrest in MCF-7 cells.

O-07

Effect 3, 3′-diindolylmethane (DIM) encapsulated chitosan nanoparticle DIM @ cs-np on human mammary cancer cell (MCF-7) by modulating biochemical and molecular markers

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3, 3′-Diindolylmethane (DIM) is a phytochemical had an extensive variety of pharmacological activities; its properties such as dissolubility and low bioavailability have impeded its clinical improvement. In this manner, it is great interest to study whether the nano for-mulation for DIM with Chitosan for an impro-ved their potential. The preparation of nano-particles by the ionic gelation technique is a viable strategy for medicating conveyance in the human mammary malignancy cell line (MCF-7). The nanoparticles synthesis and characterization by the methods of UV spec-trophotometer, Zeta Sizer, Particle size analy-zer, scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FT-IR), Thermogravimetric analysis (TG), *in vi-tro* drug release and pharmacokinetic study. Further, we scrutinize the therapeutic efficacy of DIM@CS-NP in the human mammary can-cer cell line (MCF-7) using MTT, biochemical analysis, comet assay, acridine orange/ethidium bromide staining and we-stern blotting analysis in MCF-7 cells. The encapsulated DIM spherical shape particles with their average diameter around 50–110 nm and their size were found to be greater, the drug concentration of 50 mg DIM showed high encapsulation and loading efficiency of 95.80±1.25% and 36.70±2.41% respectively. Furthermore, mammary cancer cells treated with encapsulated DIM inhibited cellular proliferation through intrinsic apoptotic signaling pathways. Hence, DIM encapsulated chitosan nanoparticles have proved to be a perfect form of drug targeted delivery in cancer treatment. The results emphasized that, this novel formulation could possibly overcome the current limitations of DIM provides a novel therapeutic regime for mammary cancer.

O-08

Evolutionary conserved genomic signatures among cancer heterogeneity

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Cancer is a complex evolutionary disease that involves the accumulation of genomic alterations proceeding through somatic evolution resulting in high degree of complexity due to its highly heterogeneous, dynamic and meta-static nature. Although cancer is curative at the early stages, most of the cancer patients are diagnosed at an advanced stage due to poor specific signs and symptoms at early stages, lack of reliable screening techniques and recurrence of the disease. Therefore, the identification of reliable and effective biomarkers is a major challenge in cancer research. The underlying mechanism and complexity of cancer can be studied with better representation using a holistic approach that focuses on the overall molecular interactions on a global scale instead of a reductionist approach that focuses

on the impact of particular genes on a disease(Koutsogiannouli et al.). The dynamic and metastatic nature of cancer can be better understood from an evolutionary perspective since cancer progression proceeds through somatic evolution driven by evolutionary forces through directional selection on clonal lineages(Shpak and Lu). Therefore, the integration of various computational approaches and genomic interpretation using the high-through-put data may help in finding reliable biomar-kers by deciphering the underlying complex processes in carcinogenesis(Tiwary). In this study, we performed a query-based gene co-expression network analysis to identify new biomarkers from the existing biomarkers. We identified overlapping pairwise interacting genes that are present across the majority of cancer. We comparatively analysed these genes to find the evolutionary conservation among the organism which either rarely get cancer or highly susceptible to cancer in the mammalian lineages. Interestingly, we found that all the genes were not positively selected in human but most of the paired genes are positively selected in cancer-resistant groups. The predictive and prognostic analysis showed that the genes can effectively classify cancer samples from the healthy sample as well as a significant impact on the overall survival rate of cancer patients in the majority of common cancer types. Moreover, the pathway analysis showed that the candidate genes are mostly in-volved in the cellular process. These results imply that the conserved paired genes confer a selective advantage under similar physiolo-gical constraints during the course of evolu-tion, therefore, they perform a similar biologi-cal function such as the cell cycle, pathway, and gene expression. Finally, we propose the identified conserved gene pairs as unified biomarkers for common cancer types.

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O-09

Evaluation of liver glycogen content in stz induced diabetic rats treated with *naregamia alata*

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Several medicinal plants are known for their hypoglycemic effects in Indian Traditional Medicine and are used in Ayurveda. The present study is aimed at evaluating the effect of methanol extract of *Naregamia alata* Weight & Arn. (Meliaceae) on liver glycogen content in streptozotocin induced diabetic rats. Methanol extract treatment showed a significant ($p<0.01$) reversal of blood glucose level, improvement in body weight and liver glycogen content in diabetic rats compared to that of control groups. The preliminary phytochemi-cal analysis revealed the presence of phenols, favonoids and terpenes in the methanol extract of *N. alata*, which might be responsible for its hypoglycemic activity by enhancing liver glycogen content. Therefore, our study concludes the possible use of *N. alata* in the management of diabetes by enhancing glycogen synthesis.

O-10

In silico Prediction of Potential Bacteri-ocin Gene Clusters in genome of probi-otic *Bacillus amyloliquefaciens* BTSS3 isolated from *Centroscyllium fabricii* (Deep sea shark) gut

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Bacteriocins are large functionally diverse group of ribosomally synthesized family of antimicrobials found in all major lineages of bacteria, which kill or inhibit closely-related or non-related bacterial strains. Antimicrobial peptides (AMPs) from bacteria are promising alternatives to antibiotics to combat enhanced antimicrobial resistance. *Bacillus amyloliquefaciens* BTSS3 isolated from *Centroscyllium fabricii* gut has been characterised for its probiotic potential and its genome sequenced. This strain also produces bacteriocin. In this study a comprehensive bioinformatics analysis of the *Bacillus amyloliquefaciens* BTSS3 genome for the presence of bacteriocin related gene clusters was done *in silico* using BAGEL4, which scans publically available genomes for potential bacteriocin gene clusters. AMPs belonging to four bacteriocin classes and the ATP-Binding Cassette (ABC) transporter proteins belonging to ABC-2 family associated with bacteriocin production were identified. These may prove to be promising antimicrobial candidates and more studies are needed to confirm the antimicrobial properties of these predicted molecules.

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O-11

Astrocyte Elevated Gene-1 *(AEG-1)* and its Downstream Targets in Primary and Metastatic Colon Cancer

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Colon cancer is the third most commonly diagnosed malignancy in both men and women, and major cause of cancer-related death worldwide. AEG-1 is identified as a metasta-sis mediating factor and it has become inten-sively studied in a large variety of cancers in-cluding colon cancer. The main aim of this re-search is to investigate the effect of silencing oncogene *AEG-1* and also to study its down-stream targets in primary and metastatic colon cancer. Experimental studies were performed on primary (SW480) and metastatic (SW620) colon cancer cell lines. Forward siRNA transfection was performed using *AEG-1* siRNA with Lipofectamine RNAiMAX. The expression levels of mRNA and protein were determined by real-time PCR and immunofluorescence analysis. Survival of cells was determined using CCK-8 assay, clonal efficiency using colony forming unit assay, apoptosis using flow cytometry analysis, migration using scratch assay, and invasion using Transwell assay on SW480 and SW620 cells. Transfection with siRNA significantly suppressed the expression of *AEG-1* gene after 24 h. Moreover, treatment with *AEG-1* siRNA had effects

on colon cancer cells and inhibited the proliferation, migration, and invasion and also induced apoptosis. Surprisingly, expression of *EXT-1*, a tumor suppressor (which is a downstream of *AEG-1*) was found to be upregulated in *AEG-1* silenced cells. Understanding the molecular mechanism underlying the role of *AEG-1* as an oncogene in colon cancer cells helps to prevent metastasis and finding a pos-sible interaction between *AEG-1* and *EXT-1* in signaling cascade might help us to establish them as prognostic biomarkers in colon can-cer.

Keywords: colon cancer, astrocyte elevated gene-1, exostosin-1, biomarker, metastasis

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O-12

Probiotic potential of yeast isolated from fermented fruits and vegetables

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Probiotics are microbial food additive which helps in bettering intestinal tract, strengthening the immune system, harmonizing the bioavailability of nutrients, decreasing the preponderance of allergy in inclined individuals. In the present study, vegetables like bitter gourd and cucumber and fruits like kiwi and amla were allowed undergo natural fermentation and probiotic yeasts were isolated using YEPD medium. The seven isolates were characterized by morphology and sugar fermentation. The probiotic potential of the isolates was assessed by acid tolerance, bile tolerance, salt tolerance, antibiotic susceptibility and anti-microbial activity. Further they were tested for antioxidant activity by DPPH assay. All seven isolates presented good tolerance towards acid, bile and salt. The isolates resisted the activity of regular antibiotics like amoxicillin, tetracycline, etc. Though the isolates did not present antimicrobial activity against gut pathogens but they compete with them and multiplied significantly. DPPH assay revealed the good anti-oxidant potential of the isolates with respect to the standard, gallic acid. The findings confirmed the probiotic and anti-oxidant properties of the yeast isolates present in fermented fruits and vegetables.

Poster Presentations

P-01

Antioxidant potency of Lagenandra toxicaria Dalz. and Ariopsis peltata Var.

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Plants are the richest source of medicine all over the world. Nowadays free radicals have occupied the attention of scientists because, free radicals easily alter the structure of protein, lipids and DNA and triggers the human diseases like cancer, diabetes and liver damage. Many synthetics drug was developed, but people are looking for plant-based medi-cine to avoid the side effects of the synthetic drugs. Present study revealed the antioxidant potential of the rhizome methanol and water extracts of the *Lagenandra toxicaria* and *Ariopsis peltata*. *Lagenandra toxicaria* metha-nol extract showed good DPPH scavenging activity (IC_{50} 477.57±3.75µg/ml) and also showed strong ferric reducing power compared to other plant extracts. The phytochemical analysis showed the presence of phenol-ics and flavonoids in both the plant extracts, which might be responsible for its antioxidant activity and these plants can be used as protective agents against oxidative stress caused by the free radicals.

P-02

Role of GATA1 and GATA1s in hematopoietic lineages

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The GATA1 protein belongs to the GATA family of transcription factors and is essential for cell proliferation and differentiation of hematopoietic and endocrine cell lineages. It consists of two zinc finger DNA binding domains and found to be more than 70% conserved. Mutations cause for the formation of truncated form GATA1s which lacks the N-terminal transactivation domain. GATA1s is less able to activate the erythroid gene expression and terminal differentiation in erythroid-megakaryocytic differentiation potential cells but an additional propensity to produce more megakaryocytes. This study aims to address the differential role of GATA1 and GATA1s in hematopoietic line-age differentiation. Based on binding profiles available for GATA1 from ChIP-Seq experiments, 297 and 156 genes were regulated by GATA1 binding in Erythrocyte and Megakaryocyte lineages respectively. In or-der to study the oncogenic potential of GATA1s, genome wide biding and the ex-pression profile of GATAs1 in Mus musculus G1ME cell line and the gene expression pro-file of GATA1 and GATA1s available with the Homo sapiens iPSC cell line were uti-lised. This integrated analysis can provide the potential role of GATA1s and its target factors in mediating the oncogenic activity.

P-03

Impact of cold plasma irradiation on reduction of Aflatoxin in the Groundnut kernel infected with Aspergillus parasiticus

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Fungal pathogens affect the quality and re-duce the yield of crop and in groundnut, inap-propriate post harvesting methods, improper handling, transportation and storage leads to growth of molds that produce mycotoxin which are carcinogenic, mutagenic and geno-toxic. Cold plasma irradiation has significant fungicidal effect on seeds that is attributed due to the generation of reactive oxygen spe-cies (ROS) and reactive nitrogen species (RNS) generated on cold plasma exposure. The present study demonstrated the efficacy of cold plasma irradiation on reduction of af-latoxin content in groundnut and elucidating the mechanism of fungal inactivation. The groundnut kernels were artificially inoculated with fungal species *Aspergillus parasiticus* and subjected to inductively coupled RF plasma of frequency 13.56 MHz utilizing the feed gas O_2 at 70W for a period of 15 minutes. The effect of cold plasma irradiation on the degradation of aflatoxin content was quantified through HPLC. Aflatoxin B_1 and B_2 content of the plasma untreated samples was 0.25 ppm and 1.23 ppm respectively whereas complete degradation of aflatoxin below the quantifiable limit of 0.1 ppm was observed in O_2 plasma treated samples. Im-pact of O_2 plasma treatment on the membrane disruption and rupture of spore coat in *Asper-gillus parasiticus* was studied using scanning electron microscope. The interaction of cold plasma on the surface of the spores causes small pores due to electroporation that results in lysis of fungal spores. The impact of cold plasma treatment on the quality parameter was assessed by determining the fatty acid profile of the treated and untreated groundnut samples through GCMS and least difference was noticed in their profile. The results of the study indicated that the effective use of cold plasma processing provides a promising source for controlling microbial diseases.

P-04

HIV-associated cancer

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This abstract is mainly focused on HIV and cancer. Fritz Balduin Lickint found the con-nection between lung cancer and smoking. In the past 30 years the scientific and medical research technologies were developed. These cannot be integrated or processed by conven-tional analytical approaches. Still lung cancer cannot be cured but it can be treated. Lung cancer is formed by uncontrolled growth of cell in tissues, it is due to smoking and some chemicals like asbestos, arsenic etc. Mainly most of the HIV patients are pretentious to lung cancer. Lung cancer can be predicted by spiral CT scan. But the patients who were in-fluenced by both cancer and HIV are treated by antiviral drugs. The patient with both dis-eases is injected by antidrug. If the patient with cancer is injected by HIV antidrug like zidovudine, he is cured from cancer but he is influenced by HIV and if he or she is injected by cancer antidrug like cyclophosphamide or vinblastine, they are cured from HIV but they are affected by cancer. Nuelasta is the best cancer treating drug. Efficacy and toxicity data for chemotherapy or radiation therapy are few and imprecise. So, surgery remains the treatment of choice but not the cure. This cause destruction of lung parenchyma caus-ing emphysema. For women who currently smoke, the chance of dying from heart dis-ease and lung cancer exceeds the chance of dying from breast cancer at the age of 40. Im-munotherapy is one of the best methods to treat lung cancer. This study purpose is a con-ventional review. Still lung cancer cannot be

cured but can be treated. So how HIV and lung cancer relate. This can diagnostic and measures against such a condition.

P-05

Synthesis and characterization of Poly-mer coated zinc oxide nanoparticles and their UV blocking efficacy using zebrafish embryo model

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Zinc oxide (ZnO) nanoparticles have pro-found use in cosmetic products as sunscreens, paints and other ultraviolet (UV) light scav-enging applications. ZnO at its nanostructure form like nanoparticles are found to be toxic and a biocompatible form with similar UV light scavenging activity is warranted. In the present study, we have synthesized ZnO na-noparticles and coated them with chitosan- a natural polymer (ZnO-CTS) and polyeth-ylene glycol (PEG) - a synthetic polymer (ZnO-PEG). The UV absorption efficacy and stability were enhanced upon coating with chitosan and PEG, compared to uncoated ZnO nanoparticles. The effect of ZnO, ZnO-CTS and ZnO-PEG nanoparticles on zebrafish embryo revealed lower deposition of ZnO-chitosan and ZnO-PEG nanoparticles atop the eggs compared to ZnO. The survival of zebrafish embryos was also studied using cumulative hatchability, and was always found to be higher in case of ZnO-CTS with respect to ZnO-treated ones. PEG coating ex-hibited better UV attenuation, but *in vivo* it induced delayed hatching. Thus, one of the reasons for better survival could be attributed to lower aggregation of chitosan coated ZnO nanoparticles on the eggs thereby facilitating the breathing of embryos. It can be thus con-cluded that chitosan coating on ZnO showed enhanced UV blocking ability and better bio-compatibility.

P-06

Structural and functional insight into the impact of Isoniazid resistant muta-tion on Mycobacterium tuberculosis InhA

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Growing concern about the difficulty in diag-nosis and treatments of drug-resistant tuber-culosis falls under the major global health is-sues. There is an urgent need for finding novel strategies to develop drugs or bioactive molecules against the global threat of *Myco-bacterium tuberculosis* (MTB). Isoniazid (INH) is a front-line drug against tuberculo-sis, it primarily targets the enoyl-acyl carrier protein reductase (InhA), a potent drug target in the mycolic acid pathway of MTB. To gain deeper insight into the impact of INH re-sistant mutation and its influence on the struc-tural dynamics of InhA, combined conforma-tional dynamics and residue interaction net-work (RIN) studies were performed. The mo-lecular dynamics investigation provided a hint about the structural changes altering pro-tein activity. The principal component analy-sis (PCA) based free energy landscape plot highlighted the highest stable part of wild-type (WT) and mutant structures. Intri-guingly, the mutation at the 78th position of InhA from its native residue valine to alanine increases the structural stability with higher NADH binding affinity. The MMPBSA based binding energy calculations confirm

that electrostatic interactions played a critical role in the binding of NADH at the binding site of InhA. The calculated binding energy score, as well as potential hydrogen bonds and salt bridge networks, proved the strong binding of mutant InhA as compared to WT. Further, the mutation potentially altered the protein network topology, thereby subse-quently affected the landscape of NADH binding. The present study is an attempt to understand the structural and functional im-pact associated with drug-resistant mutation (V78A) thus it will help design potent inhibi-tors against drug-resistant tuberculosis.

P-07

Biosynthesis and characterisation of silver nanoparticles from Aralia spi-nosa leaf extract and their antimicro-bial activity

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Aralia spinosa is a native plant distributed in Eastern North America and anti-microbial drug is produced through the extraction of sil-ver nanoparticles from the leaf. Silver nano-particles are recognized as having an inhibi-tory effect toward many bacterial strains and microorganisms commonly present in medi-cal and industrial processes. The present study was to synthesis silver nanoparticles from *Aralia spinosa,* silver nanoparticles were analyzed using UV-visible spectros-copy and SEM analysis. The antimicrobial activity at various concentration of 50 -500 was studied using agar well diffusion method for the following microbial strains *Aspergil-lus niger, A. welwitschia, E. coli, Pseudomona sp.* And *Staphylococcus sp*. Zone of inhibition was compared among bac-terial and fungal strains. The results showed the maximum zone of inhibition was obtained in the bacterial species.

P-08

Characterization of recombinant BCG strains overexpressing immunodomi-nant antigen of *Mycobacterium tuber-culosis*

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Tuberculosis (TB) is an infectious disease caused by *Mycobacterium tuberculosis* (*M. tb*). The common vaccine used for TB pre-vention is *Mycobacterium bovis* Bacillus-Calmette-Guérin (BCG), which provides pro-tective efficacy against pulmonary TB. The potency of BCG vaccine is a driving force for the development of new vaccines against tu-berculosis. The current study focusses on im-proving anti-tuberculosis vaccine by overex-pressing the TB antigens. The present study focuses on the construction of recombinant BCG overexpressing immunodominant anti-gens of *M. tb.* Rv0148 is predicted to be im-munodominant and belongs to the oxidore-ductase family and might be involved in var-ious functional categories like intermediatory metabolism, aminoglycoside drug resistance of *M. tb*. The study also focuses on the func-tional role of BCG0148 as an immunodomi-nant antigen apart from other functions. The strain displayed no difference in colony for-mation and *in-vitro* growth kinetics showing

there is increase in the growth of overexpression strain compared to wild type BCG. Further study on BCG0148 using ELISA for IL-1β, IL-6, IL-10, TNF-α cytokines showed no considerable difference in the expression of cytokines compared to control BCG. The overall study states that immunodominant an-tigen Rv0148 displays no significant role in immunogenicity. Additional studies on ani-mal model is required to validate the current results.

P-09

Effect of lamotrigine- an antiepileptic drug on viability and development in *Drosophila* epileptic *mutants*

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Drosophila has been proposed as a useful, rapid, and economical model in the preliminary screening for teratology studies. The aim of Developmental toxicology is to detect any adverse effects of xenobiotics on the pregnant female and on the development of the embryo and fetus as a consequence to exposure from starting with implantation through the entire period of development. To understand the developmental toxicity and teratogenic susceptibility on exposure to Lamotrigine-an antiepileptic drug in two different strains of Drosophila, they will be allowed to complete their development on media supplemented with various concentrations of the drugs. Developmental toxicity evaluated on the basis of hatchability, pupation, adults eclosion (viability) and mortality. Teratogenicity will be evaluated by performing a broad survey of external morphology of the adults resulting after drug treatment.

P-11

Exploring the tissue level modular assembly of SWI/SNF complex

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The chromatin architecture at the gene regulatory elements which is required for gene regulation can be achieved by the SWI/SNF family of chromatin remodelling complexes. The multi-subunit complex of SWI/SNF is formed by the assembly of around 12 subunits. The subunits show tissue-specific expression pattern and thus tissue-specific subcomplexes of SWI/SNF are formed. Also, it has been reported that the complex is arranged as submodules and understanding the SWI/SNF assembly pathway in each cell type is important for understanding the role of the SWI/SNF complex in controlling the tissue-specific expression programs. Only limited studies have reported so far on the assembly and architecture of the SWI/SNF complex. Apart from that, the modular assembly and sub-complex formation in different tissue types are not addressed so far. This study is an effort to systematically analyze the submodule architecture and assembly of the SWI/SNF complex in different tissue types and its control over tissue-specific expression programs. A data analysis strategy based on gene expression data from genome-wide expression profiling of human tissue types available with Genotype-Tissue Expression (GTEx) portal will be explored. This portal provides experimental results of RNA-Seq dataset which is collection of 17382 samples from 54 tissue types of 948 donors. Co-expression correlation analysis of SWI/SNF subunits in different tissue types can give hint on the tissue specific submodular assembly and will be explored in this study. The observations from the analysis will be presented.

P-12

An integrated analysis to identify the SWI/SNF target genes regulated by its promoter and enhancer activity

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Gene regulation mechanism in eukaryotes is highly complex and involves multiple fac-tors, including gene regulatory sequences such as promoters, enhancers and plenty of trans-acting factors, including transcription factors and other cofactors. Such a gene reg-ulatory mechanism can either induce or re-press the expression of genes. One among the regulatory sequences is enhancers that per-form their role independent of its orientation from their target promoter. The enhancer can be in the active or poised state based on the histone modifications such as acetylation and methylation happening on it and thus dictates the fate of the gene. It is known that the SWI/SNF family of chromatin remodelling complex can target enhancer sites to regulate lineage-specific differentiation apart from binding to the promoter and is found to have implications in cancer, developmental disor-ders, and other biological processes. How-ever, the detailed understanding of SWI/SNF regulatory features at enhancer sites and their target genes are not well explored. This study focuses on understanding the enhancer medi-ated gene regulation by SWI/SNF remodel-ling complex and identifying the SWI/SNF target genes. For the study, the genome-wide binding profile available for the active en-hancer marks such as H3K4me1, H3K4ac and p300 acetyl-transferase in HeLa-S3 cell line along with the SWI/SNF subunits bind-ing profile available for BRG1, BAF47, BAF155, and BAF170 has been utilized. We could identify 1637 and 891 genes that are

regulated by SWI/SNF enhancer and promoter activity respectively. Further validation of the identified target genes is performed based on the chromatin conformation capture data available from 5C and ChIA-PET experiments on the HeLa-S3 cell line. Thus, this integrated analysis aims to identify a valid list of SWI/SNF target genes, which can be further confirmed by experimental techniques.

P-13

In silico design of epitopic vaccine for chronic respiratory disease caused by *Mycoplasma gallisepticum*

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The *Mycoplasma gallisepticum* is a substantial respiratory pathogen that develops chronic respiratory disease in chickens. In spite of that, effective vaccine development for this pathogen delays because of the im-mune evasion that is caused by extensive phase variation caused by Variable lipopro-tein haemagglutin A (vlhA). The most cru-cial step for initial infection is the adhesion of *M. gallispeticum* to the host cell surface this is achieved by cytoadherence proteins such as GapA and CrmA. Control of *M. gallisepti-cum* by antibiotics is practiced in most of the poultry farms, but it has the probable risk of developing antibiotic resistance. At present tiamulin and tylosin are used in poultry farms, but recent reports suggest there is an increase in tylosin resistance in past decade. A successful vaccine is essential to address the current state of Mycoplasma infections in chickens. Recent advances in immunoinformatics allows us to exploit the available data to predict the most efficient epitopic region in antigenic proteins which further led to epitope-based vaccine development. The present study focuses on development of epitope-based peptide vaccine from cytadher-ence proteins and Variable lipoprotein haemagglutin A. Thus, with the immunoinformatics tools we predicted potential CTL epitopic regions STSETVIDY and ETGYLYFPY respectively for GapA- and vlhA cytoadherence proteins which inter-acted well with chicken BF2 alleles. Like-wise, HTL epitopes for both the proteins were also predicted: FAALISKPA and FYKLDSTKL. With the present finding we have opened up a new dimension of epitope-based vaccine design with ample therapeutic application against *M. gallisepticum* and its associated infections.

P-14

In silico toxicity assessment of mushrooms obtained from Western Ghats, Tamilnadu and their usage as potent nutrient supplement

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Malnutrition is one of the important issues to be noted. Children those who are undernourished should get a better nutritional supplement. Mushrooms could be one of the best sources, since they are most delicious food with higher nutritional value in addition it also possesses some medicinal values. The only disadvantage of mushrooms is that in some cases they are toxic and causes lethal and even fatal effects on consumption. Thus, the chief aim of the proposed work is to find out the proteins that are responsible for such ill effects and to degrade them by natural ways to make it edible.

Moreover, the work could bring out a conclusion of various potential protein sources that

are available in mushrooms to meet out the day to day protein requirement in children with malnutrition.

The work is extended to study the interaction of the proteins whether they have drug like properties and their compatibility to be consumed as a normal food material. As a conclusion the gene sequences responsible for the toxic protein is identified and reported there by to degrade them. Meanwhile the other nutritious substances shall be consumed

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P-15

Identification of miR-582-5p in macrophage cell lines infected with knockout mutant of Mycobacterium tuberculosis

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Tuberculosis is an infectious disease caused by *Mycobacterium tuberculosis (M. tb)*. The bacterium enters the host and survive using various defense mechanisms by altering the immune cells through the modulation of micro RNAs. Micro RNAs regulate gene expressions and immune responses of the host. mi-RNA's expression is one of the important strategies implemented by pathogenic bacte-ria to survive inside host immune cells. The present study focusses on the identification of novel mi-RNA in knock out mutant of *M. tb* (Rv0148). Rv0148 gene belongs to oxidoreductase family plays a significant role in various aspects such as intermediatory metabolism, stress and homeostasis of *M. tb*. By considering the functional role of gene the present study focussed on identification of miRNA biomarkers. Bioinformatic tools like miRDB, miRBASE were used to predict the list of miRNAs in Rv0148. Finally, using MiR Target we predicted miR-582-5p as a strong interaction to Rv0148. In extension to these we further infected H37Rv, Rv0148 mutant & complement strains using THP-1 cell line for the isolation of miR-582-5p. The extraction of miRNA from supernatents con-tinued with real time PCR displayed the re-duced miR-582-5p expression in mutant (ab-sence of gene) compared to wild type and the complement strain. Since, the miR-582-5p was involved in apoptosis we assume that Rv0148 also has a role in apoptosis by cross checking the miRNA expression in comple-ment strain of Rv0148.

Thus, the upregulated miR-582-5p in complement strain of Rv0148 can serve as a diag-nostic biomarker for TB infection.

P-16

Enhanced therapeutic efficacy of Ciprofloxacin encapsulated in mixed polymer nanoparticles

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A ciprofloxacin coated PLGA nanoparticles with chitosan have been used for the determination of antibacterial and antibiofilm properties. Ciprofloxacin coated PLGA nanoparticles (P2) and ciprofloxacin coated PLG nanoparticles (P3) with coating of chitosan have been compared with a control of ciprofloxa-cin solution (P1) against Enterococcus fae-calis. The ciprofloxacin coated PLG

nanoparticles with coating of chitosan was prepared by double emulsion evaporation method and surface morphology, encapsulation efficiency and drug releasing profile thoroughly studied to optimize the therapeutic efficacy. The antimicrobial and antibiofilm properties were assessed by *in vitro* biofilm inhibition assay. The drug released kinetics was studied spectrophotometrically to compare the controlled released profile of the drug *in vitro*. The P1 shows burst drug release within 1 hour whereas after 72 hours of the study P2 & P3 showed controlled release. The zone of inhibition generated by P1, P2 and P3 were also support the same observa-tion. Biofilm inhibition was figured out 60%, 70% and 90% respectively for P1, P2 and P3. Therefore, it can be concluded that the ciprof-loxacin encapsulated in PLGA-Chitosan has highest potential against Enterococcus fae-calis.

P-17

Genetic predisposition of Human Epithelial Growth Factor receptor 2 gene polymorphisms with Fibroadenoma susceptibility

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Fibroadenoma (FA) is a cancerous breast lesions, usually diagnosed in young females, where the genes, proteins and environmental risk factors contribute to the disease pathogenesis. The aim of the study was to find the association of HER 2 with FA in our population. Approximately around 120 people were enrolled in our study for both case and as well as control. DNA isolation was performed from peripheral blood lymphocytes, genotyped with ARMS-PCR method. Allelic and genotypic frequencies, Odds ratio, 95%, confidence intervals were calculated for both the variants. We used 2 different Rs id's in our study, difference in genotype frequencies of gene polymorphism was found in compar-ing with FA patients and healthy control. And from this study gene polymorphism was found to be associated with FA. As per inter-national studies it was found that HER2 is 50 % associated with FA and 50% is not associated based on 2 different rs ids. But our study was carried out in Chennai district in order to find the association of this gene with FA and it was the very first research carried out in Chennai with FA and as per our results one rs id was associated with this FA and other rs id was not associated**.**

P-18

Design and development of nanoparticle based methods for gastric cancer imaging and therapy

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Recent developments in the use of nanotechnology for designing and developing nano based products as dual-edged swords have gained tremendous importance. Literature survey indicates a significant increase in research based one nanoparticles mediated theranostics applications and also a significant work is being carried out on the use of nanoparticles to combat gastric cancer. In the past five years reseach on theranostic applications of nanoparticles have gained importance. 5-aminolevulinic acid has gained significance for imaging tumors and also for treatment.

Research in recent times is directed now-days to improve the efficacy of 5-aminolevulinic acid for diagnosis and therapy. Research on the use of nanoparticles for delivery of 5-aminolevulinic acid is underway. These studies mainly focus on either improving the efficacy of 5-aminolevulinic acid as an imaging agent or for photothermal therapy. Few studies have focused on the use of 5-aminolevulinic acid for imaging as well as for photothermal applications. Our study is focused on the use of biopolymers as nanocarriers as they achieve cell permeability and also these nanoparticles have a lot of functionalities that can be used for tagging targeting ligands and also for encapsulating drugs. In this regard, we designed an image guided targetable nanocarriers with drug/dye/nanoparticle for chemo-photo therapy of gastric cancer. The advantage and applications of using such systems against gastric cancer would be presented.

P-19

An investigation of the cytotoxicity and bactericidal ability of the commonly used pesticide triphenyltin hydroxide

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Triphenyltin hydroxide (TPTH), a commonly used pesticide causes adverse health effects in a variety of organisms including humans and is a potential contender for the environ-mental pollutant. In this study, we investi-gated the cytotoxic and bactericidal mecha-nism of TPTH. We found that TPTH inhib-ited the proliferation of HeLa cells with a half-maximal inhibitory concentration of 0.25 ± 0.05 µM and causes mitotic arrest. Im-munostaining results indicated strong depol-ymerization of interphase microtubules and perturbation of spindle apparatus with the ap-pearance of colchicine type mitosis and con-densed chromosome. Further, TPTH strongly binds to pure tubulin with a dissociation con-stant of 2.29 ± 0.15 µM and inhibited the *in vitro* microtubule assembly in the presence of glutamate as well as microtubule-associated proteins (MAPs). Docking studies along with competition studies indicated TPTH binds to the colchicine site of tubulin within an inter-molecular distance of 11 Å. DNA binding studies indicated TPTH binds to the A-T rich region of the minor groove. TPTH also inhib-ited the bacterial cell growth with MIC value of 3 µM in *B. subtilis* and 14 µM in *E. Coli* without perturbing the functions of FtsZ, a prokaryotic tubulin homolog. The present study provided adequate evidence to suggest that TPTH causes cytotoxicity in HeLa cells through DNA binding and by binding at the colchicine site of tubulin causing microtubule depolymerization and c type mitotic arrest in a similar manner as of colchicine. The results also revealed that the bactericidal mechanism of TPTH is through DNA interaction without disturbing the functions of FtsZ.

P-20

Identification of causative organism of the infectious keratitis using NGS methods

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Infectious keratitis is a devastating corneal disease, that can lead to significant vision loss worldwide. This study aims to identify and confirm the main causative organisms and microbial composition of infectious keratitis

patients using 16S ribosomal RNA (rRNA) and Internal Transcribed Spacer (ITS) sequencing. Corneal ulcer and corneal infiltrate scrappings were collected from the 14 keratitis patients randomly chosen eye for sequencing. The Illumina sequencing (Miseq) was used to sequence the 16S rDNA V3-V4 hypervariable region for bacterial sample; ITS1 and ITS2 (Internal transcribed spacer) region for fungus sample. Microbial composition and taxonomy profile of the corneal surface of infectious keratitis were investigated using Ezbiocloud and Qiime pipelines. Microbial diversity correlation and abundance among the isolates were also analyzed. Taxonomy analysis of all 14 infectious keratitis samples showed that higher abundance of Proteobacteria *(51 %),* Firmicutes (27 %)*,* Acinetobacteria (13 %) at the phylum level. At the genus and species level, *Streptococcus pneumoniae* (16 %)*, Methylobacterium extorquens* (9 %)*, Moraxella nonliquefaciens* (6 %)*, Acinetobacter indicus* (5 %), *Ralstonia pickettii* (4 %) and *Staphylococcus aureus (4%)* were detected mostly in 9 Bacterial samples. The majority of fungal phyla belonged to Ascomycota (54 %), Heterokontophyta (46 %) and Basidiomycota (0.01 %). The *Pythium insidiosum* (99 %) *and Aspergillus flavus* (95 %) were the main organism found in all 5 fungal samples, followed by *Aspergillus nomius* (8 %) *Cladosporium halotolerans* (5 %) *and Colletotrichum gloeosporioides* (3 %). 16S ribosomal RNA (rRNA) and Internal Transcribed Spacer (ITS) gene-based sequencing methods proved to be better diagnostic method compared to conventional culture-based techniques in keratitis patient samples. In addition, multiple causative organisms can be detected.

P-21

Sequentially distant but structurally similar proteins exhibit fold specific patterns based on their biophysical properties

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The Three-dimensional structure of a protein depends on the interaction between their amino acid residues. These interactions are in turn influenced by various biophysical properties of the amino acids. There are several examples of proteins that share the same fold but are very dissimilar at the sequence level. For proteins to share a common fold some crucial interactions should be maintained despite insignificant sequence similarity. Since the interactions are because of the biophysical properties of the amino acids, we should be able to detect descriptive patterns for folds at such a property level. In this line, the main focus of our research is to analyze such proteins and to characterize them in terms of their biophysical properties. Protein structures with sequence similarity lesser than 40% were selected for ten different subfolds from three different mainfolds (according to CATH classification) and were used for this analysis. We used the normalized values of the 49 physio-chemical, energetic and conformational properties of amino acids. We characterize the folds based on the average biophysical property values. We also observed a fold specific correlational behavior of biophysical properties despite a very low sequence similarity in our data. We further trained three different binary classification models (Naive Bayes-NB, SupportVectorMachines-SVMand Bayesian Generalized Linear Model-BGLM) which could discriminate mainfold based on the biophysical properties. We also show that among the three generated models, the BGLM classifier model was able to discriminate protein sequences coming under all beta category with 81.43% accuracy and

all alpha, alpha-beta proteins with 83.37% accuracy.

P-22

Invitro study of growth and inhibition of the struvite crystals by using the stem of the *Alpinia galanga*

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To investigate the inhibitory effect of stem of *Alpinia galanga* on the growth of struvite crystals. Struvite crystals were grown by the single diffusion gel growth technique *in vitro* and evaluate the inhibition efficiency of methanol extract of stem of the *Alpinia galanga*. Materials used for this work are Powder of stem of *Alpinia galanga*, Soxhlet apparatus, Thin layer chromatography and Column chromatography. With the help of hot extraction method, the sample will be collecting from soxhlet apparatus. Then the primary and secondary metabolites have been seperated by using thin layer and column chromatography. After that, quantitative and qualitative test will take place. Flavonoid, Tannin, Saponin, Alkaloids, Phenols and Terpenoids were there in the sample. Among these, Terpenoids have controlled the growth of struvite crystals. The grown crystals were characterized by Fourier Transform Infrared Spectroscopy (FTIR) to confirm the functional groups and Powder X-Ray diffraction (XRD) methods for further confirmations. With an increase in the concentration of methanol extract of stem of *Alpinia galanga*, the weight of the formed crystals were gradually reduced from 1.56g to 0.31g in struvite crystals, respectively. Intake of Modern medicines for kidney stone is causing side effects such as low blood pressure, dizziness an tiredness. This plant medicine has been developed with an intention to reduce the side effects.

P-23

Isolation and characterization of *Arachis hypogea* nut shell protein and its effects on macrophage activation and anti-leishmanial potential *in vitro*

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Leishmaniasis is the neglected tropical disease which is caused by *Leishmania species*. The severe form leishmaniasis is the visceral leishmaniasis (VL). It is caused by the *Leish-mania donovani. L. donovani* mainly affects visceral organs i.e. spleen, liver, and bone marrow. Macrophages are the key effector cells which are making household environ-ment for the parasites. Anti-VL drug treat-ments have a lot of side effects which leads to fatal. In this study, we have isolated crude *Arachis hypogea* protein (AHP) from the agro by-products of *A. hypogea* nutshell and possible anti-VL responses have been studied *in vitro*.
Crude protein isolated and fractionized by the size exclusion chromatography, yielding two protein peaks named as fraction-1 (AHP-F1) and Fraction-2 (AHP-F2). The presence of a protein in the Native PAGE and SDS PAGE identified as 28 kDa molecular weight protein. The MALDI-TOF analysis confirms that

purified AHP-F2 molecular weight is 28 kDa. MS / MS analysis showed the protein's similarity with that of Mannose-binding lectin with the support of MASCOT software. The isolated AHP-F2 increased nitrite generation and proinflammatory cytokines (IFN-γ and IL-12) in murine macrophages significantly ($p<0.01$) indicating the potential immunomodulatory impact against visceral leishmaniasis. Importantly, AHP-F2 (0.5µg/mL) showed better parasite clearance by 70.7% compared to the other fractions ($p<0.001$). Hence, the isolated AHP-F2 can be used as immunomodulatory anti-VL biomolecule that may be considered as one of the novel treatment approaches for visceral leishmaniasis in near future.

P-24

Tuning of GFPs folding and stability using hydroxyproline and DOPA incorporation

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Green fluorescent protein (GFP), a natural bioluminescent having the ability to emit fluorescence when they are exposed to ultraviolet to blue light range. This discovery made a huge embark in the various field such as cell biology where they are used to stain live organism and they also can be used as reporter gene in the recombinant DNA technology. In order to increase its life span and stability various method of mutation are used and one such mutation lead to development of GFPhs protein. This was obtained by two mutations in wild GFP (S65G and S72A). By assembly PCR, this was again mutated (35 mutations) to produce highly stable GFP (GFPhs) with the increased stability without the loss of functional properties. Although mutation have increased stability yet they are up to lim-ited level. In order to overcome this a new concept of introducing non-canonical amino acid was introduced. These amino acids are chemically synthesized compounds and they are not coded in m-RNA yet they have a sim-ilar property as that of natural amino acids. In this study we investigate the structural stabil-ity, folding and function of GFPhs protein by incorporating two non- canonical amino acid (hydroxyproline incorporation instead of proline and DOPA instead of tyorosine) via global incorporation.

P-25

Human body - on – chip platform enables *invitro* prediction of drug behaviour in humans

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Drug development is an extremely arduous and costly process, and failure rates in clini-cal trials that test new drugs for their safety and efficacy in humans remain very high. According to current estimates, only 13.8% of all tested drugs demonstrate ultimate clinical success and obtain approval by the Food and Drug Administration (FDA). There are also increasing ethical concerns relating to the use of animal studies. As a result, there has been a world-wide search to find replacements for animal models. Organ Chips are microfluidic culture devices composed of a clear flexible polymer the size of a computer memory stick, which contains two parallel hollow channels that are separated by a porous membrane. Organ-specific cells are cultured on one side of the membrane in one of the channels, and vascular endothelial cells recapitulating a

blood vessel line the other, while each channel is independently perfused with cell type-specific medium. The porous membrane allows the two compartments to communicate with each other, and to exchange molecules like cytokines, growth factors, and drugs, as well as drug breakdown products generated by organ-specific metabolic activities. It might be possible to create a human "Body-on-Chips" by transferring fluids between the vascular channels of many different types of Organ Chips to mimic blood flow, and as-sessing drug PK/PD behaviors across the en-tire linked system. A highly modular Body-on-Chips platform, which is enabled by an engineered "Interrogator" instrument that can culture up to 10 different Organ Chips, and sequentially transfer fluids between their en-dothelium-lined vascular channels to mimic normal human blood flow between the differ-ent organs of our body. We use a computa-tional scaling method to translate data ob-tained from drug experiments involving 3 dif-ferent types of fluidically-linked Organ Chips to their respective organ dimensions in the real human body. The approach is able to quantitatively predict changes in drug levels over time, as well as organ-specific toxicities, that have been previously measured in human patients. The Interrogator instrument enables us to culture, perfuse, and link many living human cultured tissues in a multi-Organ Chip system, as well as add and sample the me-dium in a fully programmable way, using the device's robotic liquid transfer capabilities, while continuously monitoring tissue integ-rity with an integrated microscope. In this study, we serially linked the vascular chan-nels of eight different Organ Chips, including intestine, liver, kidney, heart, lung, skin, blood–brain barrier and brain, using a highly optimized common blood substitute, while independently perfusing the individual chan-nels lined by organ-specific cells. The instru-ment maintained the viability of all tissues and their organ-specific functions for over three weeks and, importantly, it allowed us to quantitatively predict the tissue-specific distribution of a chemical across the entire system.

P-26

Ameliorative efficacy of Psidium guajava l. on spermatogenesis in diabetic induced albino rats

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Insulin resistance syndrome is one of the metabolic dysfunctions that plays a crucial role in the pathogenesis of type 2 diabetes mellitus. Sustained hyperglycemia has been linked with many complications including altera-tions in reproductive system and infertility with poor semen quality. Improvement of hyperglycemia through herbal remedy is an effective approach in treating diabetes. This study investigated the protective role of *Psidium guajava* L. (PG) leaf extract to combat diabetes-induced adverse effect on spermatogenesis. Matured male albino rats were divided into four groups: Rats of the first group were served as normal controls. Second group were streptozotocin (STZ)induced dia-betic group , third and fourth groups were di-abetic rats treated with glibenclamide (GLB) at a dose of 5mg/kg/b.w and PG leaf extract (PGL) at a dose of 150mg/kg/b.w for 8weeks. Rats were checked for fasting blood glucose level, testosterone level and epididymal sperm charcteristics. A diminuition activity in STZ group was reflected here by signifi-cant lower values of serum testosterone level, organ weight, sperm count and elevated blood glucose level. Administration of PGL extract resulted, significant ($p<0.05$) recov-ery in blood glucose and hormonal levels than GLB with the highest percentage of normal sperm count. The study proves that, PGL ex-tract possesses a potential role against

diabetic reproductive disorders which may be due to its antioxidant activity and its ability to normalize spermatogenesis.

P-27

An *insilico* approach to model *TAGAP* gene and study the interaction with vit-amin D Receptor-Retinoid X receptor complex

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T cell activation Rho GTPase activating protein (TAGAP) gene expression is higher in Rheumatoid arthritis patients compared to healthy individual. Since Vitamin D Receptor Element (VDRE) sequence is present in the regulatory region of TAGAP gene, it could be targeted by vitamin D dependent Vitamin D Receptor (VDR)-Retinoic acid X Receptor (RXR) heterodimer complex and regulate the TAGAP gene expression. It is studied that Vitamin D treatment could possibly down regulate TAGAP gene expression. This reduction of TAGAP gene expression could prevent further severity of RA disease condition. In this study calcitriol which is a vitamin D small molecule was evaluated for its ADMET property by pkCSM and as it obeys Lipinski rule of drug likeness it could be used as a drug .The VDR structure was docked with RXR protein using patch dock gave an atomic contact energy (ACE) score as 285.23 and further this complex was docked with VDRE region of TAGAP gene modeled us-ing 3d Dart server , the ACE value obtained from patch dock was -304.29 and followed by NUCPLOT was used to find out the interaction between the gene and the protein complex. Thus, this study aims to show that the interaction exists between VDR-RXR and VDRE sequence of TAGAP gene so calcitriol could be used to enhance the down-regulation of TAGAP gene to suppress the severity of RA disease.

P-28

Molecular docking studies for identification of novel drug against lactamase in antibiotic resistant bacteria

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Antibiotic Resistant Bacteria is evolving as the most inevitable threat to the medical field all over the world. These bacteria develop resistance against antibiotics using various mechanisms like, ß-lactamase enzymes, efflux pumps and etc. In which ß-lactamase enzymes are the most employed antibiotic resistant mechanism. Specifically, in which CTX-M ß-lactamase is resistant to most of the cephalosporin drugs as they inhibit the ß-lactam ring in these drugs. Currently there are numerous ß-lactamase inhibitor drugs available. The ß-lactamase inhibitors like Clavulanic acid, sulbactam, Tazobactam Avibactam. These drugs have different efficacies. It is important to identify the novel drug against this enzyme. So, the three-dimensional structure of CTX-M 15 were predicted using Swiss model Server and the interaction be-tween the CTX-M site and these different types of ß-lactamase inhibitor drug is evalu-ated using molecular docking. Based on the docking score and binding pattern, the tazo-bactam is the best inhibitor against the se-lected targeted enzyme compared to other ß-lactamase inhibitors

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P-29

Cloning and expression of Organophosphate Hydrolase (OPH) gene from methl parathion degrading *Enterobacter cloacae*

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Organophosphates (OP) are extensively used worldwide in agriculture and public health practices for controlling pests, which have caused toxicological and environmental nuisances on non-target organisms due to its high persistence. Degradation of organophosphorus compounds has also alternatively explored to reduce its persistence in the environment, which has attracted considerable attention. Bioremediation of organophosphate pesticides using bacteria is serious concern as it is efficient in converting the toxicants in to innocuous byproducts. In this study, *Enterobacter cloacae* subsp. *dissolvens* was isolated from pesticide contaminated soil from paddy field, which could effectively degrade methyl parathion to p-nitrophenol. The gene corresponding to Organophosphorus Hydrolase (OPH) was cloned using a PCR cloning strategy based on the known OPH gene of *Enterobacter cloacae* SDM. Sequence BLAST result indicated this gene has 92% similar to OPH. The OPH gene is 975 bp long with G+C content of 63% that encodes a polypeptide of 324 amino acids with a molecular weight of 42 kDa. Further, OPH gene was successfully cloned in pET-30b (+) vector, expressed in *E. coli* and purified. The recombinant enzyme hydrolyzed methyl parathion with a total activity and specific activity of 740 U. mL^{-1} and 287 U.mg^{-1}, respectively. These results highlight the potential of this bacterium to be used in the bioremediation of pesticide contaminated environments.

P-30

Social interaction in a uropathogenic *E. coli* biofilm during stress

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Uropathogenic *Escherichia coli* (UPEC) is the major cause of urinary tract infections (UTI) in both community and health care settings. UPEC strains possess a superfluity of both structural and secreted virulence factors that contribute to their capacity to cause infection. Biofilm formation in UPEC are the major cause of chronic and recurrent urinary tract infections (rUTI). Bacterial subpopulations within biofilms have competing interests and needs. Deciphering the mechanisms of interactions within these microbial communities shows how bacteria can cooperate with each other to sort out a form of social conflict. The mechanism of biofilm to stress does not evolve from a specific gene or from a first-rated cell type, it emerges from the zestful of the community. In this poster, we will discuss the social behaviour between the biofilm variants of UPEC with response to the antibiotic stresses.

P-31

Effect of BPMS22 antigen in M2 to M1 macrophage repolarisation

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Macrophages are the phagocytic immune effector cells which possess extensive functional dynamicity. Due to this property, macrophages are characterized as M1 (classical activation) or M2 (alternate activation), and in their respective polarized states the cells exhibit different phenotypical status coherent to their function. During leishmanial infec-tion macrophages get polarized to M2 pheno-type as the parasite possess the ability to sup-press the anti-leishmanial immune effector responses. The objective of this study is to validate the potential of a novel marine BPMS22 antigen induced M2 to M1 re-polarization of the macrophage to treat visceral leishmaniasis. BPMS22 antigen was purified by GFC and affinity chromatography and was used to treat the BALB/c derived macrophages *in vitro*. We observed that BPMS22 significantly ($p<0.05$) decreased the FIZZ-1, YM-1, CD206, Arg-1 and increased IL-1β, IL-12 mRNA expressions in IL-4+IL-10 in-duced M2 macrophages. Interestingly, BPMS22 significantly ($p<0.05$) decreased the FIZZ-1, YM-1, CD206, Arg-1; signifi-cantly ($p<0.05$) increased iNOS2, IL-12, IFN-γ, TLR-4, TLR-9 mRNA expression in AG83-infected murine macrophages beside the decreasing parasite load in it. Altogether, BPMS22 holds its ability to repolarize the cy-tokines (IL-4+IL-10) stimulated and *L. do-novani* infected M2 macrophages to M1 phe-notype *in vitro*. Decrease in parasite burden after treatment with BPMS22 indicates the acceleration of the parasite killing by enhancing the macrophage effector functions. The alignment of these results might open up new perspectives of BPMS22 in immunotherapy.

Keywords: BPMS22, M1 macrophage, M2 macrophage, repolarisation, Leishmaniasis

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P-32

Structural analysis on Cu/Zn SOD1 of human and *Wuchereria bancrofti* to identify the structural hotspot towards the development of novel structure-based drug discovery for lymphatic fil-ariasis

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Lymphatic filariasis, commonly called as elephantiasis is majorly caused by the nematode, *Wuchereria bancrofti*. These parasitic worms are transmitted into host through mosquitoes and majorly the infections are asymptomatic but still cause subclinical damage to lymphatic system, kidneys, with proteinuria and haematuria. The human immune system employs different types of cells and molecules to eliminate the parasites from body, which causes oxidative stress due to release of reactive oxygen species (ROS) from the cells of immune system. However, the worms survive the cytotoxicity caused by ROS despite localized in the lymphatic vessels, which might be due to its efficient antioxidant system. So, our study focused to investigate structure and dynamics of antioxidant enzymes of *W. bancrofti* to develop new small inhibitor molecules.

In the preset study we investigated the structure and dynamics of one of the antioxidant enzymes of *W. bancrofti*, Cu/Zn superoxide

dismutase (WB-SOD1). The three-dimensional structure of monomeric WB-SOD1 was modelled from its amino acid sequence using I-TASSER server and the modelled protein was energy minimized to remove the steric clashes and stereochemical quality was checked by Ramachandran Plot and finally it was compared with human wildtype SOD1 (H-SOD1) (PDB ID: 1HL5). The modelled WB-SOD1 and experimentally solved H-SOD1 were subjected to molecular dynamics simulations (MD) using GROMACS 5.1.2 package and GROMOS96 53a6 force field for 50 ns, at three different temperatures (300K, 310K and 320K). The structural changes of WB-SOD1 and H-SOD1 were an-alyzed in terms of change in potential energy, RMSD and RMSF of backbone atoms, radius of gyration and secondary structures at three different temperatures. These results showed that both WB-SOD1 and H-SOD1 structures are stable and intact throughout the 50 ns simulation at 300K, 310K and 320K and secondary structures analysis showed stable β-sheets for both human and WB-SOD1 during entire simulation. The position of the Cu and Zn metal ions was studied and the results showed that both the metal ions are stable with their metal biding site residues. Further analyses are in progress to identify the unique struc-tural hotspots in WB-SOD1 to identify the small molecule inhibitors that could help to treat elephantiasis.

P-33

Structural studies on novel DrwH protein from *Deinococcus radiodurans* to understand the desiccation tolerance mechanism

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Desiccation is a common problem for all life forms. Some species have evolved with special pathways to tolerate anhydrobiosis for certain period of time. *Deinococcus radiodurans,* a polyextremophilic bacterium, amongst very few species of bacteria that have developed special mechanisms to sus-tain under extreme conditions like desicca-tion and radiation. DrwH, a *D. radiodurans* protein, has showed desiccation tolerance ability even when expressed in *E. coli* bacte-rium. However, the underlying mechanism of DrwH activity is yet to be understood. In this direction, the present study is focused to explore the structural aspects to understand the mechanism of DrwH activity, using computational methods such as molecular dynamics simulation and molecular docking. The three-dimensional structure of DrwH protein was modelled using fold recognition via threading by I-TASSER server and validated. Analysis of DrwH amino acid sequence using SignalP 5.0 suggest the presence of a signal peptide (1-16 amino acids) at C-terminal region and a conserved WHy domain, which is con-sistent with the earlier studies. The modelled DrwH protein was subjected to molecular dy-namics (MD) simulation using GROMACS 5.1.2 package and GROMOS96 53a6 force field for 50ns. RMSD of backbone atoms, root mean square fluctuations (RMSF), ra-dius of gyration (Rg) of the protein were an-alysed using GROMACS. Further secondary structural changes during the simulation period were analysed using STRIDE web server. During simulation, it is observed that the signal peptide gradually lost its secondary structure (α-helix) but the WHy domain which is made of β-sheets, remained very sta-ble. Further, molecular docking was per-formed to investigate the affinity and binding domain/region (WHy domain) of DrwH with peptidoglycan layer. Binding of DrwH with peptidoglycan subunits might help the

peptidoglycan layer to maintain its stability during anhydrobiosis. Detailed results will be presented.

P-34

Competition and cooperation between population variants during motility in *E. coli*

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Urinary tract infection (UTI) is among the most common infectious diseases of humans and is the most common nosocomial infec-tion in the developed world. UPEC is the ma-jor causative agent of the infection. Biofilm transform independent cells to specialised cell population. Biofilm is essential for estab-lishment of the infection and increases the bacterial pathogenicity in the host. When Uropathogenic *Escherichia coli* were plated on the congo red media, we observed hetero-geneity which shows red, white and hetero colony variants. Sugar source in the media is one of the vital factors which determine the existence and survival of the population. When subjected with glucose in the media the ability of the variants to quench the glucose is analysed. And swarming motility is stud-ied.

P-35

Ligand-receptor interaction studies of amino acids with lacto peroxidase

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Molecular insights of protein developed by evaluating ligand-receptor interaction pro-vides a platform for analysis of potential lig-ands for selective isolation of target mole-cule. Affinity chromatography is a new age technique of chromatography. Ligands of high affinity are bound to the stationary phase of the column for selective entrapment of tar-get protein. The Receptor in present study (crystal structure of Bovine lactoperoxidase at 2.3 A^0 resolution) was retrieved form Pro-tein DataBank (PDBID-2GJ1) (1). Various ligands such as Amino Acids (Cysteine, His-tidine, Tyrosine, Leucine) and Metal ions (Copper, Cobalt and Cadmium) are retrieved from the PubChem database (Pubchem mole-cule reference) (2). They are retrieved in the Three-dimensional SDF file format and fur-ther SDF files are converted to PDB file for-mat using UCSF Chimera molecule visuali-zation software (3). Autodock Vina was used for Docking the protein with ligand molecule. Lactoperoxidase and the tyrosine docked complex is having the highest binding affin-ity with an energy of -5.7kcal/mol. The resi-dues such as ARG-333, ASP-94, ASP-98 are present in common undergoing various inter-actions with the ligand molecule. Hence, they might have some importance and may act as a binding site.

P-36

Mechanistic insights in to attenuation of metal, fatty acid and ligand binding activity due to binding pocket modifi-cation of HSA: a case study with cys34 glycation

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The binding pockets in albumin are inevitable for its extraordinary ligand binding proper-ties. Minor changes in the binding pockets would affect the binding affinity of their re-spective ligands. Generally, glycation leads to covalent modification of residues (Argi-nine, Cysteine and Lysine) in proteins under hyperglycemic condition. These modifica-tions ultimately lead to diabetic complica-tions. Methylglyoxal (MG) is one of the strongest glycating agent, which is derived from the glucose metabolic pathway. The Cys34 in albumin plays a major role in anti-oxidant and radical scavenging property. The Methylglyoxal modification of cysteine leads to formation of carboxyethyl cysteine (CEC), which has adverse effects on fatty acid bind-ing, esterase activity and metal binding prop-erty in albumin. Here we have focused on *in vitro* studies of esterase and metal binding ac-tivity of MG glycated albumin and molecular dynamics (MD) of *in silico* glycated Cys34 albumin. The MD analysis of Cys34 modified albumin gives plausible changes in the sur-face area of the respective sites such as multi-metal, fatty acid binding and esterase activity sites. The influential effect of Cys34 modifi-cation in human serum albumin leads to steric hindrance site occurrence in the respective ligand binding sites of albumin and also ex-plains insights of impairment.

P-37

An investigation on the anti-microbial and anti-biofilm efficacy of semi-synthetic imidazole derivatives

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The rising numbers of antimicrobial resistant pathogens that are associated with nosocom-ial infection has become one of the most chal-lenging problems of the healthcare system. The spread of ESKAPE pathogens has dra-matic impact on the global economic and clinical sectors as they are associated with high mortality and morbidity rates. *Entero-coccus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter bau-mannii, Pseudomonas aeruginosa*, and *En-terobacter* spp are the six nosocomial patho-gens that comes under the acronym ESKAPE and exhibits multidrug resistance and viru-lence. Even the most effective drugs are ren-dered ineffective due to the emergence of multidrug resistant (MDR) and extensively drug resistant (XDR) bacteria that has been provoked by the persistent use of antibiotics. The ESKAPE pathogens also share the ability to form biofilm by attaching to tissues (e.g., surgical sites, medical implants), which makes ESKAPE infections difficult to pre-vent and treat with current antibiotics and of-ten require surgical procedure. In order to stay ahead of the ever-rising drug resistant ESKAPE pathogens, there is an urgent neces-sity to restock our armamentarium of antimi-crobials.

In this study, we have evaluated six synthetic compounds for their anti-microbial activity against ESKAPE pathogens. One of the com-pounds showed inhibitory against *Enterococ-cus faecium and Staphylococcus aureus*. This compound is further evaluated by the micro-dilution method and minimum inhibitory concentrations were determined. In addition, anti-biofilm assay showed that the compound is capable of inhibiting *Enterococcus* faecium biofilm.

P-38

Disrupting of uropathogenic *E. coli* (UPEC) biofilms by Glycolipids derived from Renewable resources

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Urinary tract infections (UTI), which are common worldwide with about 150 million cases per annum is known to be caused predominantly by UPEC bacteria. UPEC Chronic infection of bacteria are caused by biofilms and it is also a survival strategy of the pathogens in a non-host environment. Several amphiphilic molecules have been used in the past to potentially disrupt bio-films. Herein, we report a facile synthesis of glycolipid-based surfactant from renewable feedstocks in good yield. Interestingly, these glycolipids self-assemble into gel in highly hydrophobic solvents and vegetable oils. The potential application of these self-assembled glycolipids to disrupt preformed biofilm was examined against UPEC. It was observed that glycolipid 6c was effective in disassembling UPEC biofilm. Altogether, the supramolecu-lar self-assembled materials, either as gel or as surfactant solution could be potentially used for surface cleansing in hospital envi-ronments or the food processing industries to effectively reduce pathogenic biofilms.

P-39

Mitigating the quorum sensing mediated virulence of the phytopathogen *Ralstonia solanacearum* by an agricultural byproduct

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Ralstonia solanacearum is a soil borne plant pathogen which causes wilt disease in economically important crops of the *Solanaceae* family in tropical and temperate regions. It is the second most common bacterial plant pathogen which causes bacterial wilt in more than 50 plant families and decreases the production of solanaceous crops. The pathogen enters into the plants vascular tissue through damaged roots or root opening by chemotaxis. Once the bacteria enter into the host, it multiplies rapidly throughout the plant and blocks the xylem vessels by the production of enormous amount of Exopolysaccharide which is mediated by quorum sensing. This results in decreased sap flow in xylem vessels and causes wilt disease. As biofilm formation is the major virulence factor in *R. solanacearum*, it is necessary to identify natural biofilm inhibitors to mitigate virulence of this bacterium. Hence in the present work, the anti-biofilm potential of phytochemical compound gallic acid (GA) isolated from an agricultural byproduct (cashewnut shell) was investigated against *R. solanacearum.* GA will be an effective eco-friendly alternative to mitigate *R. solanacearum* virulence.

P-40

Biofilm formation in Vulvovaginal candidiasis (VVC): A neglected etiology

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Despite therapeutic advances, Vulvovaginal candidiasis (VVC) continues to be a global problem. It is an important health disorder among women belonging to the reproductive age group. It is caused due to biofilm mediated drug resistant *Candida* species. Absence of a rapid and simple diagnostic test results in misleading of diagnosis. *C.albicans* is the most common pathogenic species among *Candida* sp. causing this type of infections. However, over the last two decades, non albi-cans Candida (NAC) species which includes *C. glabarata*, *C. tropicalis* and *C. auris* have emerged as the leading causative agents of VVC. So appropriate identification of *Candida* sp will pave way for a better treatment and drug administration. The increased use of azoles and use of intrauterine devices, results in increase in number of causative agents for VVC. So, the aim of this study is to analyse the species distribution of Candida among infected women at the molecular level, their biofilm forming ability and their resistance profile for standard antifungal drugs which are in high need to study for the further treat-ment and eradication of biofilms caused by *Candida* species.

P-41

Exploratory data analyses on cancer genomics data

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Cancer is one of the major causes of death across the world. On performing exploratory data analyses on cancer genomics data, we can bring about a change in the way of treat-ing cancer in a more efficient manner. This study aims to find gene expression patterns, corresponding to different drug responses in cancer patients. The gene expression data and drug response data were retrieved from The Cancer Genome Atlas (TCGA) using RTCGA package in R. Drug response data was integrated with the gene expression data. Both breast and skin cancer subtypes had suf-ficient drug response information and so those two cancers were selected for the study. Relation between the drug response and the gene expression for the chosen cancers were analysed. The interdrug variability was investigated using principal component analysis, heat map, correlation circle, hierarchical clustering and box plot. In case of breast cancer, CEACAM6 and CEACAM6 were identified to make significant contribution in different drug responses. Similar pattern was observed in skin cancer for the genes KRT1, KRT5 and TYRP1.

P-42

Disturbed glucose metabolism in rat neurons exposed to cerebrospinal fluid obtained from multiple sclerosis subjects

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Perturbed glucose metabolism is implicated in neurodegenerative diseases. However, lit-tle is known about its role in multiple sclero-sis (MS) pathology. We therefore hypothe-sized to look for perturbance, if any, in ex-pression of genes implicated in glucose me-tabolism in neurons treated with cerebrospi-nal fluid (CSF) of MS patients. The effect of possible factors in CSF on healthy demyeli-nated granule neurons isolated from rat cere-bellum which are able to regulate axonal de-struction-repair, and make a stable remye-lination and functional recovery possible was studied. Identification of these mechanisms involved in axonal degeneration-reconstruc-tion may shed light in understanding MS pro-gression and /or prognosis.We used a cellular model with primary cultures of unmyelinated granular neurons from rat cerebellum. These primary cultures were treated with the CSF of distinct clinical forms of MS including oli-goclonal band of IgG + and IgM type –relap-sing remitting MS, primary progressive MS and neurological controls. Global gene ex-pression profiling using microarray techno-logy was performed.The present research shows a significant variation in gene expres-sion catalyzing essential steps of carbohy-drate metabolism in healthy neurons exposed to CSF of MS patients as compared to neu-rons exposed only to culture medium.These data suggest that factors in CSF of MS patients cause a disturbance in metabolic gene(s) expression and demonstrates that MS seems to be associated with metabolic im-pairment.

P-43

Detection of substance levels

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Substance abuse is when the use of a particu-lar substance, like a drug/ alcohol/ marijuana, in amounts or by methods that are harmful to the individuals and the ones around them. Re-cently it has been discovered that substance abuse can cause problems not only in the in-dividual, but also to their progeny. These sub-stances have been found to cause certain her-itable phenotypic changes in the individual and hence are harmful to their progeny. It is also known to be the cause of several mental and psychotic disorders in the individual. In order to identify if a person is under the influ-ence of alcohol or drugs, we give their urine or blood sample to the laboratory. When we do this, the individual comes to know that they have been caught and tries to stop using them, but then relapse back in most of the cases. But, drugs and alcohol in the body can even be detected using sweat/ saliva/ tears/ hair samples too. Using a simple device, which can be used by anyone; literate, illit-erate, young and old; it can be identified if a person is under the influence of any of the il-legal substances without them knowing. Thus, the individual can be helped to over-come the substance abuse disorder com-pletely.

P-44

Theoretical study on electrochemistry, chemical reactivity and opto-electrical properties of biogenic amine neurotransmitters

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Biogenic amine neurotransmitters (dopa-mine, epinephrine, norepinephrine, histamine and serotonin) are associated with major neurological activities in human. They have structural as well as biological similarities and therefore one may interfere in others' activities. To understand the bio-physiological effect and neurotoxicity of the oxidized and photo-excited species of these neurotransmitters, we studied theoretically, the electrochemistry, chemical reactivity and opto-electrical properties, at the molecular level using density functional theory (DFT), density functional reactivity theory (DFRT) and time-dependent density functional theory (TD-DFT). We observed that calculated ver-tical ionization potential (VIP) for individual molecule (gas phase) follows the order: serotonin (1) < epinephrine (2) < norepinephrine (3) < dopamine (4) < histamine (5), which in-dicates that removing a single electron verti-cally in gas phase becomes much more diffi-cult when we approach from (1) to (5). The calculated electron affinity (EA) for all the neurotransmitters under study is positive. It indicates that addition of single electron to the neutral molecule is not favourable in gas phase unlike the electronegative atom (supported by the electron density distribution of the frontier molecular orbitals). The calculated NRP (non-adiabatic reduction potential) values reflect that cationic species of seroto-nin and histamine are respectively energetically most and least stable and that of catecholamines are in between. The most stable cations might be reactive further in the biological systems. The electrophilicity index represents the overall attractive tendency of the neurotransmitter as a whole molecule towards the electron density. The electrophilicity is the highest for histamine and lowest for serotonin and the catecholamines in between. Calculated electrostatic potential identified the localization or accumulation of specific charges (either positive or negative) in the neurotransmitter molecules. All the neurotransmitters under study can absorb UV light. Histamine is excited with the lowest wavelength (~195 nm) of light and norepinephrine is excited with the highest wavelength (~278 nm) for the lowest allowed transition (singlet to singlet). The analysis of natural transition orbitals (NTOs) for the lowest allowed transition predicted that the neurotransmitters under study are photo-toxic, since LUNTOs attain π-anti-bonding character, which is dominated in the aromatic ring. This is supported by the bonding parameters (bond length, bond angle and dihedral angle) of the neurotransmitters at the first singlet excited state. In addition, we observed that the trend of oxidation potentials of the neurotransmitters in aqueous phase (using non-reaction-based method) follows the reverse order of VIP (in gas phase) having the highest oxidation potential (~1.1 V) for histamine and the lowest (~0.72 V) for serotonin. This indicates that removing single electron becomes much easier in aqueous phase when we go from (1) to (5). This may be due to the combined effect of solvent polarity (environmental effect) and dipole moment (inherent property of the mol-ecule) of the neurotransmitters.

P-45

Synthesis and characterization of PVA capped Zinc oxide nanoparticles nano particles

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Zinc oxide is a wide band gap semiconductor with large exciton binding energy at room temperature. The combination of superior physical, chemical, biological, electrical, optical properties of the zinc oxide (ZnO) material at the nanoscale make them a promising material in the field of nanoscience and technology. Zinc oxide nanomaterial finds potential applications as gas sensors, electronic devices, photocatalysts, light emitting diode, medical and dental materials, pigments, UV protecting coatings, antibacterial agent and ingredients in pharmaceutical, cosmetic products and so on. It is possible to control the aggregation, agglomeration and enhance the stability and biological activity of zinc ox-ide nanoparticles by surface modification. The surface modification of zinc oxide nanoparticles can be achieved by capping agents such as polyvinyl pyrrolidone (PVP), polyvinyl butyral (PVB) or polyvinyl alcohol (PVA). Surface capping by PVA will be help-ful in controlling the particle size and crystal-linity of the zinc oxide nanoparticles.

In our present experimental study, we have prepared the PVA capped zinc oxide nanoparticles using chemical precipitation method. Zinc nitrate hexahydrate has been used as precursor salt and sodium hydroxide has been used as reducing agent. The formation of spherical shaped PVA capped zinc oxide nanoparticles has been confirmed by scanning electron microscopy measurements. We are going to study the biological activity of the synthesized PVA capped zinc oxide na-noparticles such as anti-bacterial and the an-giogenic property.

P-46

Investigation on energy efficient stirred split cylinder reactor using var-ious test fluids: hydrodynamic aspects

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Chemical reactors are vessel were reaction process is carried out. It is the heart of chemical process industries in which the raw materials are converted into products. These reactors are classified into various types. Among those reactors, split cylinder reactor is one such kind of energy efficient multi-phase reactor, which is used in large scale application due to their simplicity in construction and to enhance the efficiency. The main objective of this work is to study the hydrodynamic aspects of stirred split cylinder reactor for air-water system. Here water is replaced using different test fluids like nano fluids and viscous fluids. The effect of pressure drops, gas holdup, power on various fluids was investigated. Under various concentration Gas holdup was observed at different air flow rates, different bed height and with stirring. It is observed that gas hold up increase with increase in concentration also with increase in superficial air velocity. It was also noticed that holdup was more with stirrer than without stirrer. Mass transfer Co-efficient increases with increase in superficial velocity and stirrer speed.

P-47

Separation of nitrogen from air using zeolite 13 for the reduction of NOx

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Automobile emission consists of NO_x, SO_x and CO_2. In this, NOx, emission re-sults in smog formation and acid rain, so it's important to reduce NO_x in atmos-phere. Many researchers had done work on reduction of NOx after the combustion process using catalytic convertor but our studies focused on source reduction of Nitrogen from air using a selective zeolite as a adsorbents with maximum surface area. By the process of alkali fusion followed with hydrothermal treatment Zeolite 13x was synthesized using a natural clay bentonite. By varying bentonite - NaOH ratio and calcination temperature, different zeolites were prepared and analyzed for maximum capacity. The synthesized zeolites were characterized by SEM Analysis for morphology, BET for surface area and TGA for thermal stability. This investigation elucidate zeolite 13x has the maximum adsorption capacity of 68% at 8-9 bar so it can be used as cost effective adsorbent for NO_x reduction.

P-48

Simulation of gold-silver bimetallic na-noparticles in water

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The bimetallic nanoparticles composed of two different metals possess interesting tunable properties leading to possible applications in optics, sensors, catalysis and health science. The properties of the bimetallic nanoparticles can be tuned in terms of shape, size, structure and chemical composition. The structure of the bimetallic nanoparticles is characterized by the distribution and organization of two metals and it can be either random, mixed, segregated, core-shell or multishell pattern depending upon the preparation method, mixing ratio, atom size and particle size. The

bimetallic nanoparticles with the combination of gold and silver will be of great advantage due to their excellent biocompatibiltiy, unique optical, photo-thermal, catalytic, chemical and bio-chemical properties.

In the present study, gold-silver bimetallic nanoparticles of three different mixing molar ratios (2:1, 1:1 and 1:2) and gold & silver monometallic nanoparticles have been simulated to investigate their structural features, thermal and hydration properties. Molecular dynamics simulations have been performed for all the five systems in water under iso-baric-isothermal ensemble at room tempera-ture and atmospheric pressure. The force field parameters for gold and silver atoms have been taken from the literature. The core-shell model is followed for initial configura-tion of the bimetallic gold-silver nanoparti-cles. The stable structure of gold-silver nano-particles has resulted from the stronger inter-actions between gold and silver atoms. The specific heat capacity value of the bimetallic gold-silver nanoparticles was found to in-crease linearly with the increase in the per-centage of silver. The increase in the

percentage of silver might have increased the phonon density resulting in the enhancement of specific heat capacity. There is no significant difference in the hydration property of gold-silver bimetallic nanoparticles with respect to the mixing molar ratio. But we have observed little difference in the hydration property between monometallic gold, silver nanoparticles and bimetallic gold-silver nanoparticles. The tunable specific heat capac-ity values of gold-silver bimetallic nanoparti-cles and their hydration property may be har-nessed for technological and biological appli-cations.

P-49

Coconut shell based bottles as a replacement for single use plastic water bottles

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Just like the air we breathe and the water we drink, the plastic bottles have also become ubiquitous in nature. For so long, we have been throwing them away, without giving an ounce of thought. As a result, these plastic products, having major toxic pollutants are pouring into the world's water system, damaging our once pristine ecosystem. Despite this being perhaps the highest profile environmental issue in years, the movement is still in its infancy and has yet to become mainstream. Therefore, there arises a dire need for replacement of SINGLE USE PLASTIC BOTTLES to save the invaluable marine eco systems from complete degradation.

In India, almost 95% of the farmers own lands filled with coconut trees and yet, they are unable to utilize their market potential due to their lack of income from coconut husk, pith and shell. Our project demonstrates the use of coconut shells to produce water bot-tles, which would replace the existing plastic water bottles. In spite of being a waste, coco-nut shell is high on strength and has a density of 1.6 g/cm3. Coconut Shell Powder (CSP) has a unique combination of features includ-ing high lignin content, making it more weather resistant, and low cellulose content enabling low moisture absorption. From a feasibility and availability standpoint, coco-nut shells are also cheap, renewable, have less abrasion to machine, and to top the chart, are environment friendly.

At first, the coconut shells are sundried and then pulverised into powder. The obtained CSP is now uniformed to the required size by the seiving machine. Then, the CSP is mixed with suitable amount of binders like guar gum and xanthan gum and moulded to a bottle shape container. A final coating of sugarcane wax and chitosan is given for hydrophobicity and anti-microbial activity respectively. The highlight of our project is that no harmful chemicals or fumes are used/produced during (or) after the process. Furthermore, our project mainly focuses on waste management and thereby most of the materials used are agro-waste (coconut shells, sugarcane wax). CSP bottles can contribute significantly to saving our environment and can minimize the harmful impacts that plastic bottles have cre-ated to our world.

P-50

Machine learning algorithms in electronic health records

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Electronic health records contain large amounts of longitudinal data that are

valuable for biomedical informatics research. The application of machine learning is a promising alternative to manual analysis of such data. Some approaches to modeling temporal data rely on extracting single values from time series; however, this leads to the loss of potentially valuable sequential information. In this study, novel representations of temporal data in electronic health records are explored. These representations retain the sequential information, and are directly compatible with standard machine learning algorithms. The explored methods are based on symbolic sequence representations of time series data, which are utilized in a number of different ways. The proposed method creates representations that better account for the temporality of clinical events, which is often key to prediction tasks in the biomedical domain.

P-51

Treatment of Tannery Effluent using a polymeric carbon composite

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Treatment of Tannery Effluent is done using a Polymeric Carbon Composite that consists of Chitosan, Bentonite, Graphene Oxide are the adsorbents that are used to remove the to-tal Chromium content present in the Effluent. The adsorbents are characterized using vari-ous methods such as Scanning Electron Microscope (SEM), Energy-dispersive X-ray spectroscopy (EDS) to analyze the structure of the Composite, Brunauer-Emmett-Teller Analysis (BET) to study the surface morphology of the composite and Fourier Transform Infrared Spectroscopy (FTIR) to study the composition of the composite. The Continuous Treatment Process is done by packing Intalox Saddles coated with Polymeric Carbon Composite in a Catalytic bed reactor.

P-52

DSSC based on extracted vegetable dyes

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Solar cells are an alternative renewable energy source which is potentially viable to replace fossil fuels, at least partially. There's been extensive work going on in the next generation solar cells. Dye sensitized solar cell (DSSC) is one such energy source in the photo-electrochemical cell family. Compar-ing with conventional solar cells, DSSCs are a promising class of photovoltaic cells with the capability of generating green energy at low production cost since no vacuum systems or expensive equipment are required in their fabrication. Initially, previous works were done using platinum electrodes as counter electrodes. Due to economic reasons it was optimized by replacing the counter electrodes with other metal inert electrodes. Graphene oxides are one such example which is inexpensive but their efficiency needs to be optimized. Progressively biologically derived extracts are used for sensitizers in place of inorganic dyes for further feasibility. An ideal

photo-electrode has to achieve moderate thickness, good light transmittance, high degree of roughness and good electrical connection between the dye particles and the electrode layer. In the present work, Dye-sensitized solar cells (DSSC) are fabricated using TiO_2 as the photo-electrode along with Graphitic Carbon Nitride (GCN) as an electron affinitive layer to enhance the forward reaction, along with plant based extract used as the photo-sensitizer for better combination with TiO_2 particles on top of Fluorine doped Tin-Oxide (FTO) conductive glass substrate and (I_3^-/I^-) is used as redox couple.

P-53

Metal supported on fibrous nanosilica KCC-1 catalyzed synthesis of benzothi-azole derivatives under solvent-free conditions

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Benzothiazoles have been prepared by one-pot condensation ssof 2-aminothiophenol and aldehydes in the presence of metal supported on fibrous nanosilica (KCC-1) under solvent-free reaction condition have been proposed. The benzothiazoles derivatives were identified through elemental analysis and melting point measurements and characterized by FT-IR, 1H-NMR, 13C-NMR spectroscopic methods.

P-54

Phytoremediation of Tannery effluent using *Elodea canadensis* in a constructed wetland

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One of the major contributors of pollution is the effluent coming out from the tannery industries. Tannery effluent is rich in Chromium, which is highly carcinogenic. Research works were done and various treatment methods were studied. Phytoremediation is the simple and effective approach to treat the tannery effluent. In the present work, phytoremediation using the plant species *Elodea canadensis* in constructed wetland was studied. To evaluate kinetics of adsorp-tion and degradation of contaminants the phytoremediation is carried out in batch mode using the synthetic effluent of hexavalent Chromium of different concentrations namely 2.5 ppm, 5 ppm and 7.5 ppm. The treated effluent from constructed wetlands were collected in various intervals of time and characteristics like Biological Oxygen Demand (BOD), Chemical Oxygen Demand (COD), pH, Turbidity, Conductivity, Total Dissolved Solids (TDS)and Chrome content were studied. The plant growth characteristics like in simulated effluent was compared with the plant growth characteristics in fresh water. The distribution of Chromium in soil and plant parts was analyzed. The results obtained from this work confirmed that plants will grow in the Chrome environment and re-duction of contaminants was witnessed.

P-55

Benzimidazole ornamented pyrazoles through molecular hybridization approach: design, synthesis, biological evaluation and molecular docking studies

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In 21st century, cancer is static a problem in non-communicable disease. Cancer is a comprehensive collection of causes considered by the unprecise growth of irregular cells that can spread to parts of the body. According to WHO, predictable to rise in global cancer from 22.2 million by 2030 indicates popula-tion growth. Benzimidazole is a well-known as aromatic heterocyclic moiety and its similarities are hopeful platforms in medicinal chemistry through interest in the therapeutic areas. Pyrazole and its by-products were broadly used as insect killer in agrochemical division and studied for years their broad-spectrum biological actions, including insecticidal, acaricidal, antibacterial, herbicidal activity and antifungal activities. The pyrazole derivatives bearing benzimidazole nucleus, 6a-6j has been accomplished via multi-step synthetic strategy. Spectral and physical techniques have been used to establish the structures of the same. Among them, a hybrid possessing para-nitrophenyl moiety connected to pyrazole scaffold (6a) exerted the highest anti-inflammatory activity which is superior to the standard diclofenac sodium. While ex-ecuting DPPH radical scavenging activity, a para-bromophenyl unit integrated at pyrazole structural (6i) exhibited the highest activity among the hybrids examined. Besides, evaluation of anticancer potency of the synthesized hybrids reveals that the one fluorophenyl unit tethered at pyrazole nucleus (6h) showed the highest activity against the pancreatic cancer cells investigated such as SW1990 and AsPCl. Considerable binding affinity between B-cell lymphoma and the hybrid 6h has been reflected while performing molecular docking studies (-8.65 Kcal/mol). The out-comes of the investigation expose to con-struct more potent biological agents besides for further biological evaluations.

P-56

The effect of the crystallographic form of MnO2 on the kinetics of oxygen reduction reaction and oxygen evolution reaction

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The energy storage devices are essential to provide a continuous supply of power. Among various energy storage devices, zinc-air battery (ZAB) has received significant attention as it is cost-effective, environmentally friendly, exhibits high energy density, uses cost-free fuel, and zinc is earth-abundant[1]. Besides, the fabrication of ZAB is easy and does not require cleanroom facilities. However, the performance of electrically rechargeable ZAB depends on the kinetics of reactions occurring at the cathode, i.e., oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). Bifunctional electrocatalysts are required to mitigate the sluggish kinetics of ORR and OER[2].

Owing to the availability of precursors and better catalytic stability than precious noble metals, transition metal oxides are studied widely as electrocatalysts. Herein, the effect

of the crystallographic form of MnO2 on ORR and OER is reported. Five different crystallographic structures of MnO2, namely, α-, β-, γ-, δ-, and λ-MnO2, are synthesized by a hydrothermal method with similar textural properties. Among them, α-MnO2 exhibits the lowest onset potential and highest limiting current for both ORR and OER. The details of this study will be discussed in the presentation.

P-57

Development of metal free bifunctional nanocatalyst

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For zinc- air battery lack of bifunctional electrocatalyst motivated to develop highly ac-tive, low cost bifunctional electrocatalyst. Different electrocatalyst such as metal-based electrocatalyst, metal oxide based electrocatalyst, carbon based electrocatalyst are used. Among various carbon-based catalyst, ordered mesoporous carbon has special features such as high surface area, unique pore structure which makes as better candidate in the field of catalysis, electrochemistry and en-ergy related applications. In the present work, ordered mesoporous carbon was synthesized by using ludox as hard template and carbonized at different temperature such as 600 °C to 900 °C. Morphology and mesoporosity was confirmed by microscopic and nitrogen adsorption-desorption studies. Chemical composition analyzed by X-ray photo elec-tron spectroscopy and Fourier transform in-frared spectroscopy. It is found that synthe-sized carbon at 900 °C shows high surface area and activity towards ORR and compared with commercial Pt/C.

P-58

Experimental investigation on vanadium pentoxide nanoparticles

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Vanadium oxides have generated increasing scientific and technological interest due to their rich, diverse, structural, physical, chemical properties, low cost, simple synthesis process and abundant resources. Among the family of vanadium oxides, vanadium pentoxide is the most stable compound with the highest oxygen concentration. Vanadium pentoxide has a layered structure and weak Van der Waals interaction exists between the layers. This make them a good intercalation material. It possess advantages such as mixed valence state, excellent optical, electrical properties, higher accessible surface area and high-energy density. So vanadium pentoxide nanoparticles have broad range of applications such as electro-optic and electrochromic devices, high capacity lithium batteries, supercapacitors, catalysis, gas sensors, solar cells and photocatalytic reactions. In addition to many applications, vanadium pentoxide nanoparticles also have been found to exhibit magnetic properties. In literature antiferomagnetism has been observed in vanadium pentoxide nanoparticles due to oxygen vacancy.

In this study, we report the preparation of vanadium pentoxide nanoparticles by thermal method. Bulk vanadium pentoxide was used as the starting material. The formation of vanadium pentoxide nanoparticles has been confirmed by scanning electron microscopy measurements. We are going to investigate the magnetic properties of the prepared

vanadium pentoxide nanoparticles using vibrating sample magnetometer measurements.

P-59

Biopolymer functionalized metal nano-particles for detection of adulterants in milk

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Milk is one of the easily adulterated products. The reasons for adulteration of milk include the demand-supply gap, perishable character, low purchasing capabilities, and lack of suitable tests for adulteration. Adulteration of milk is a global concern, more so related to the economics of procurement. With protein content in milk chosen as a criterion for quality, adulteration with products that mimic aminoacids has come to the fore. The health consequences of adulterants raised concern on the robustness of its screening and quantification methods. There is a lacuna with several of the screening methods with respect to application or sensitivity or selectivity. With the development of sophisticated devices such as UV-Vis spectrometer, Raman spec-trometer etc. There is a need for the develop-ment of sensors that would enable detection of adulterant in milk. In this work, metal nanoparticles have been synthesized on a biopolymer template, employing the polysaccharide as a reducing agent and stabilizing agent. The interaction of adulterant with nanoparticles was studied using UV-Vis spectroscopy. Nanoparticles were characterized using UV-Vis Spectroscopy, FT IR, DLS and TEM.

P-60

Production of amphiphilic surfactant molecule from *Saccharomyces cerevisiae* MTCC 181 and its protagonist in nanovesicle synthesis

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Microbial expel nurture medicinal sciences in various dimensions. Though surface active compounds from microbes are being applied in several areas, their biodegradability and amphiphilic properties outspread greatly in therapeutic sector especially in improving drug delivery. The current work transmits on applicability of biosurfactant produced by *Saccharomyces cerevisiae* in nanovesicle synthesis. The organism was proficient in producing biosurfactant using groundnut oil as a carbon substrate and the chemical struc-ture of the surfactant moiety was predicted using FTIR, HPTLC and GCMS analysis. Biosurfactants were further employed in nanovesicular synthesis in composition with cholesterol and the vesicles were further characterized for shape, surface charge, size, using SEM and Zeta potential measurements. The surfactant from *Saccharomyces cerevisiae* displays emulsification property and its amphiphilic structure was proficient in nanovesicles with desirable shape, size and stability for drug delivery. The study was effectively made on the vesicle forming ability of the biosurfactant from *Saccharomyces cerevisiae*. Glycolipid of this yeast appears to support nanovesicle formation and this formulation can be exploited for better drug entrapment and release kinetics in the field of Pharmaceutical sciences. This is the first

prospect reported on extracellular secretion and nano application of biosurfactant from Saccharomyces cerevisiae.

P-61

Using electricigens as alternative energy source by rDNA technology

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Portable Electronics such as Cell phones, Laptops and Computers have produced a surge in Battery development. The use of Lithium Ion Battery technology as our energy source is insufficient for our current reliance of Technology improvement. So, it is im-portant to concentrate on alternative energy source for all Electronic gadgets. There are Geobacter microorganism's species which are efficient in converting Chemical energy into Electrical energy. These organisms can act as our reliable and sustainable energy source. In various Geobacter species bacteria, G. Sulfurreducens KN400 can produce high-est known current density in pure culture. The possibility of adopting this organism to pro-duce even higher current densities are being evaluated. Currently, these bacteria are using organic waste as electron source to produce electricity. Cable bacteria is also another effi-cient electricity producing bacteria. Tailoring the genetic material of Geobacter sulfurre-ducens KN400 with Cable bacteria species using rDNA technology can result in most ef-ficient hybrid production which leads to gen-eration of more sustainable and feasible en-ergy generation. Replacing organic waste with Methane, Ethanol and water as electron source can increase the performance of these bacteria to greater extent. These Microbial Fuel Cells (MFC) are the future energy source.

P-62

Niosomal nanoformulation of rhodamine improves ROS quantum yield and inactivates MDR bacteria

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Multi-drug resistance (MDR) are becoming the major challenge, recently due to the resistance exhibited by them to the conven-tional antibiotics. Alternative therapeutic techniques are warranted to overcome this problem and are now being exploited by many researchers. One of the current strate-gies is photodynamic therapy (PDT) that uti-lizes light and photosensitizers for the gener-ation of reactive oxygen species. In the pre-sent study, we have engineered nano-encap-sulated Rhodamine 6G (R6G) in niosomes for the improvement of ROS quantum yield and dependent therapeutic efficacy. The syn-thesized noisome encapsulated R6G was characterized using different photophysical tools. The hydrodynamic diameter of nio-somes encapsulated R6G was determined 52.69 nm and the singlet oxygen quantum yield was calculated by iodide method. The singlet oxygen quantum yield was deter-mined to be 0.51 in niosomal R6G which was much higher than that of R6G in water (0.203). The outcome of our study confirmed that the niosomal nano-formulated R6G can act as a potential agent for Photo dynamic inactivation of MDR microorganism.

P-63

Development of RPA-LFD based detection of Shigella in environmental water samples

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Shigellosis is an infectious bacterial disease caused by the genus shigella which develop diarrhea, fever, and stomach cramps. Development of a rapid detection method for shigella in human is critical due to its low bacterial load requirement for initiating the infection. Recombinase Polymerase Amplification (RPA), an isothermal rapid DNA amplification technique which can be coupled with Lateral Flow Dipstick (LFD) is used in the current study to develop a rapid detection method. ipaH7.8 gene is a conserved gene present in the bacterial genome and the virulence plasmid of shigella. Primers tagged with Biotin and the probe tagged with FAM in the 5' end makes it possible to detect the presence of the target DNA through a lateral flow dipstick. In the current study, the ipaH7.8 gene is amplified using PCR, cloned into pGEM-T vector and transformed into E. coli TOP 10. Further experiments were done using the transformed colonies of ipaH7.8 transformed E. coli TOP10. The RPA condi-tions were optimized for the ipaH7.8 gene. Various optimization such as least time re-quired, optimum temperature, LFD runtime and the results are validated using spiked wa-ter samples and environmental water sam-ples. The currently available rapid detection method for shigellosis takes 55 minutes using LAMP whereas RPA-LFD method takes only 30 minutes. The sensitivity of the method was assessed where the DNA load was assessed. Only 1fg of DNA was required to allow the detection which is a necessity

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P-64

Disparities in the physiognomies of sol-vothermally synthesized Barium Stannate (BSO) nanoparticles mediated using Ethylene Diamine

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The ratio variations in the solvent functionality and its significant differences in the synthesized BSO nanoparticles were discussed in the present work. The crystallographic structure, morphology, composition, optical and Photoluminescence properties were analysed using various characterization techniques. The x-ray diffraction (XRD) analysis of the synthesized samples reveals the formation of cubic structure. The SEM analysis shows an elongated cubic structure is obtained for hydrother-mally and partly EDA solvent BSO whereas flawless cubic structure is ob-tained for full EDA concentrated BSO. The EDAX microstructural analysis con-firms the basic elements such as Ba, Sn and O without any trace of impurities. A wide bandgap of 3.18eV, 3.26 eV and 3.20eV was obtained for the samples by UV-vis spectra and the PL spectrum ex-hibit peak at 442nm, 440nm and 441nm re-spectively.

P-65

Facile hydrothermal synthesis of Zn_2SnO_4 nanoparticles and its characterization

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Zinc stannate (Zn_2SnO_4) is a typical n-type ternary semiconductor and has been employed as an important multifunctional material due to its tunable work function, band gap energy, high surface area and robust struc-ture. In the present work Nanosized Zn_2SnO_4 (ZTO) particles were synthesized via simple hydrothermal process. The structural, mor-phological and compositional properties of the prepared sample were investigated through X-Ray diffraction (XRD) and Field emission scanning electron microscope (FESEM with EDS). The cubic ZTO sample without any impurity phase was prepared at 200ºC for 8 hours and its optical properties were characterized through UV-DRS and Photoluminescence studies. The as prepared raw sample exhibits crystallite size of 14nm and band gap of 3.8eV which was found to be blue shifted as compared to that of the bulk (3.6eV). Room temperature photolumines-cence spectrum showed emission bands at 425nm and 446nm. The obtained results ex-hibit better crystallinity and pure phase when compared to that of the samples prepared at longer duration

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P-66

Biocompatible core-shell nanostructures for dual-modal contrast in magnetic resonance imaging

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The presented work is based on the design and synthesis of core-shell nanoparticles for generating dual-mode contrast in magnetic resonance imaging (MRI). To achieve this objective manganese ferrite nanoparticles (MNFs) were synthesized and the surface was coated with mesoporous silica ($mSiO_2$). The coating of the MNFs with $mSiO_2$ helps to reduce the toxic effect of the manganese ions and also improves the stability and solubility of the magnetic nanoparticles. It is also observed that the mesoporous shell acts as a reservoir for the water molecules and thus plays an important role in the enhancement of the image contrast. Hence the thickness of the shell was optimized to generate better con-trast and the same was investigated by em-ploying characterization studies such as UV-Vis spectrophotometry, X-ray diffraction, vibrating sample magnetometer, Fourier transform infrared spectroscopy and particle size analysis. The role of mesoporous silica in reducing the toxicity of the manganese ions was assessed by MTT assay on HepG2 liver carcinoma cells. The assay revealed that the mesoporous silica-coated manganese ferrite nanoparticles ($mSiO_2$@MNFs) showed a higher percentage of cell viability than the bare nanoparticles.

P-67

Differentially expressed miRNA signatures as prognostic biomarkers in breast and cervical cancer

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Breast cancer is the most frequent cancer and Cervical cancer is the fourth most frequent cancer in women with an estimated 570,000 new cases in 2018 representing 15% and 6.6% of all female cancers (WHO)

respectively. This cancer is especially prevalent in developing countries, claiming the second highest incidence and the third highest death rate of all malignancies. Conventional treatment of cervical cancer involves surgery and chemo-radiotherapy, but these therapies are generally effective only in the early stages of the disease and approximately half of cases persist or recur despite these treatments. Biomarkers with high specificity and sensitivity for cervical and breast cancer are still lacking, thus the identification of novel biomarkers for cervical cancer screening is important, as such biomarkers would support early diagnosis, prediction of disease progression, and outcome improvement. In recent years, the relationship between miRNA and cancer has become a research focus. Tumor initiation and progression is related to clearly aberrant expression of specific miRNAs, which thus have the potential to serve as biomarkers for the disease. The aim of this study was to identify the differential patterns of miRNA expression between cervical adenocarcinoma tissues and matched normal cervical tissues by analyzing the TCGA breast and cervical cancer miRNA-Seq omics data. We have identified a panel of four

significantly overexpressed or downregulated miRNAs in each of the cancers of interest. Their prognostic utility value is being determined. The evaluation of the prognostic value of differentially expressed miRNAs would help identify and construct a miRNA signature which could be used as a panel of prognostic biomarkers.

P-68

Synthesis, characterisation and optoelectronic applications of nano structured Cobalt doped Zinc Oxide thin films

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Cobalt (Co) doped Zinc Oxide thin films were prepared on a glass substrate for several concentrations by sol-gel technique. The films were evaluated using Energy Disper-sive X-ray Spectroscopy (EDS), Scanning Electron Microscope (SEM), X-ray Diffrac-tometer (XRD) and Ultraviolet Spectroscope (UV). The EDS result shows the particles present in the thin films. The SEM result re-veals that as concentration of the dopant in-creases the intermolecular space decreases and conductivity increases. The XRD pattern shows a dominating peak (002) indicating c-axis oriented wurtzite hexagonal nature crys-talline structure. The UV-Vis spectrum shows that the minimum range of absorbance occurs at the visible region. All these proper-ties show that the prepared films can used as Transparent Conducting Oxides (TCO's) in solar cells, Light Emitting Diodes (LED) and other opto-electronic applications.

P-69

An ethno- scientific view on heritage rice – Mapillai samba

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As the awareness and health consciousness of people are rekindled, the wings of 'Organic' and 'Traditional' take flight for 'Healthy Liv-ing'. Mapillai samba, a heritage rice variety is being popularised as 'Bride groom rice va-riety' symbolising masculinity in Tamil nadu, India. As a part of making a best choice of strong and healthy Bride groom, a larger boulder stone called 'Ilavatta kal' need to be

lifted up by the competing young men to be chosen as the 'Bride. As a rural Tamil culture, the overnight soaked supernatant water of rice is called as 'neeragaram'. The compet-ing bachelors drink the" Neeragaram of Mapillai samba' in the early morning of the competition day which imparts instant enrgy and strength to be the winner of the tile as 'Mapillai/Bride groom'. The rice is claimed to impart physical and mental strength to a person while consuming this traditional her-itage over a period of time. In Sangam era, it is treated as royal dish which has been served for guests of royal families. Various ancient Tamil literatures, have specifically men-tioned about goodness of this variety drawing our scientific attention.

An ethno-scientific study including physico-chemical composition of such significant traditional variety has been analysed and the richness of this variety has been characterised. The grains of Mapillai samba have been characterized to be 'Medium class' with length L/W ratio of 2.56 (Unpolished) and 'Bold grains' with L/W ratio of 2.36 (Pol-ished). The bold grains of Mapillai samba has Amylose content falling under the class of 'High'there by imparting energy with soft gel consistency. The protein content is apprecia-bly high compared to the conventional hy-brids. Moreover, the GI is reported to be low making it suitable for anti-diabetic nutritional consumption recommendations. An insight into deeper perspective on the Ehtno-scien-tific aspects of Mapillai samba will be dis-cussed.

P-70

Eco-friendly supplementation of nutritional requirement for sustainable sug-arcane crop production

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In our research we were keen on exploring the endophytic bacterial niche within the sugarcane plant which could significantly contribute to the plant's nutrient status, through various plant growth promoting mechanisms such as biological nitrogen fixation, mineral bio-dissolution and phytohormone production. In this context we obtained twenty-three putatively endophytic bacterial isolates from sugarcane plant samples and screened them in order to supplement the sugarcane plant's nutrient requirement, in an eco-friendly manner, with an intention to combat the rising hazards due to ample application of chemical fertilizers. Among the 23 isolates, *Stenotrophomonas* sp. ESR 21 showed maximum production of total N (15.0 ± 0.01 mg g^{-1} of malate) and maximum nitrogenase enzyme activity (782.4 (±0.7) n mol C_2H_4 released h^{-1} mg^{-1}protein) and also showed maximum phytohormones production such as; IAA (19.2 (±0.1) µg ml^{-1}), GA (13.3(±0.08) µg ml^{-1}) and cytokinin (4.5(±0.2) µg ml^{-1}). Isolate *Pseudomonas oryzihabitans* ESS 13 showed maximum phosphate solublization efficiency (244.3(±0.5) %); and showed maximum phosphatase activity (8.1(±0.05) µg of PNP released ml^{-1} day $^{-1}$). Thus, the endophytic bacterial isolates; *Stenotrophomonas* sp. ESR 21 was selected for diazotrophic potential and for phytohormones (IAA, GA and Cytokinin) synthesis; and *Pseudomonas oryzihabitans* ESS 13, was selected for mineral bio-dissolution potential. The phylogenetic tree was constructed using the closely related strains to the two elite endophytic bacterial isolates *Stenotrophomonas maltophilia* ESR 21 (KU050688), *Pseudomonas oryzihabitans* ESS 13 (KT184485) and their taxonomical position in the bacterial kingdom was observed. The two elite endophytic bacterial

isolates showed growth compatibility and plant growth promotion activities under co-inoculated conditions. The capability of the two elite endophytic bacterial inoculants to colonize the aseptic sugarcane plantlets was evidenced by microscopic studies.

In a vision to supplement plant nutritional requirements and ensure sustainable growth of sugarcane crop, these two elite endophytic bacterial inoculants were individually formulated into wettable powder which showed higher shelf life of 20.94 log cfu g^{-1} up to one year, irrespective of the inoculant formulated. The maximum plant growth response was achieved with the treatment of single node chip buds of sugarcane (Co 86032) with 250 g ha^{-1} of formulated products. Thus, we could utilize the plant-endophytic bacterial interaction, by standardizing the entire process of endophytic bacterial inoculants development from isolation to formulation, suiting the plant genotype, for achieving sustainable growth and yield improvement in sugarcane.

P-71

Protein fabricated collagen gold nanoparticles from poutry offal and its anti-microbial activity

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Gold nanoparticles (AuNPs) are extensively employed in bio-nanotechnology because of their unique properties and multiple surface functionalities. AuNPs are promising candidates for designing novel biomaterials and they find extensive applications as carrier for drugs, in treating cancer, during X-ray imaging, and many more. Currently, eco-friendly method of green synthesis of nanoparticles (using microbes and extracts of plants) is in practise. Bottlenecks such as stability failure, accumulation of toxic compounds due to the phytochemicals of the flora are also factors to be considered. Thus, a sensible alternative of choosing a protein of animal origin may possibly overcome the concerns mentioned. Collagen plays a pivotal role as it is the major structural and fibrillary protein existing at 25% of the overall available protein. The global collagen industry showcases increas-ing demand that cannot be satisfied with the conventional sources. Poultry offal's like feathers, entrails, and internal organs from slaughterhouses, which on proper management are good raw materials for collagen extraction. In the present study, collagen is extracted from poultry slaughter wastes, which is characterized using UV-Visible spectroscopy, Fourier Transform Infrared spectroscopy (FTIR), and circular dichorism (CD). The collagen thus obtained is used for the synthesis of collagen- gold nanoparticles (C-AuNPs). The C-AuNPs were characterized through colour change, observing the characteristic peak for AuNPs in the UV-Visible spectrum, FTIR and Energy Dispersive X-ray spectroscopy (EDX). The C-AuNPs were found to exhibit antibacterial activity against gram-positive and gram-negative bacteria. The study will be extended for checking the anti-fungal activity of the C-AuNPs.

P-72

Incorporation of unnatural amino acid into protein for industrial application

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Lipases are one of the important enzymes used in various industries like diary, oleo-chemical, pharmaceutical, cosmetic, deter-gent and medical applications. Industrial pro-cesses use different solvents and harsh condi-tions such as high temperature and pressure will affect the enzyme stability, activity and affinity etc. Hence, next generation protein engineering paves a way to improve quality of such enzymes through unnatural amino acid incorporation. Here we developed a fluorotyrosine incorporated (fluorinated) en-zyme with better structural stability which can be used for efficient esterification reac-tion. Hence the congener enzyme may act as a better biocatalyst for numerous applica-tions.

P-73

Studies on synthesis of multifunctional catalyst from Kaolin

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Zeolites are crystalline, microporous, alumi-nosilicate materials with a three dimensional fully cross-linked open framework structures that form a uniformly sized pores of molecu-lar dimensions which is extensively used for cracking, isomerisation, alkylation, etc. These catalysts are mainly used in hydrocar-bon processing. Kaolin, a natural clay mate-rial contains high silica and alumina which can be used for precursor for zeolite. N-pro-pyl amine is an organic template is used for impregnation of acid sites. Hydrothermal synthesis is carried out in a Teflon lined hy-drothermal reactor at various temperatures for various time intervals. The suitable cata-lyst is selected based on acid sites and it is supported with silicon dioxide. The morphol-ogy of catalyst is studied by SEM analysis. The FT-IR data is used to determine the acid site concentration and also the temperature stability of catalyst is determined by TGA analysis.

P-74

Hydrogen sulfide and its roles in *Saccharomyces cerevisiae* in a winemaking context

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The rotten-egg odour of hydrogen sulfide (H2S) produced by the yeast *Saccharomyces cerevisiae* has attracted considerable research interest due to its huge impact on the sensory quality of fermented foods and beverages. To date, the yeast genetic mechanisms of H2S liberation during wine fermentation are well understood and yeast strains producing low levels of H2S have been developed. Studies have also revealed that H2S is not just a by-product in the biosynthesis of the sulfur-containing amino acids, but indeed a vital molecule involved in detoxification, population signalling and extending cellular life span. Moreover, polysulfides have recently emerged as key players in signalling and the sensory quality of wine because their degradation leads to the release of H2S. This review will focus on the recent findings on the production of H2S and polysulfides in *S. cerevisiae* and summarise their potential roles in yeast survival and winemaking. Recent advances in techniques for the detection of

H2S and polysulfides offer an exciting opportunity to uncover the novel genes and pathways involved in their formation from different sulfur sources. This knowledge will not only provide further insights into yeast sulfur metabolism, but could potentially improve the sensory quality of wine.

P-75

Synthesis and characterization of ternary nanostructures for supercapacitor application

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Reduced graphene oxide (rGO) integrated with iron oxide nanoparticles (α-Fe_2O_3/rGO) composites with different morphologies were successfully obtained through the in-situ synthesis reflux condensation method. The graphitic carbon nitride (g-C_3N_4) with iron oxide (α-Fe_2O_3/rGO/g-C_3N_4) composites have been prepared by a one-step hydrothermal method using cynuaric acid and melamine. Success-ful fabrication of metal oxides with carbona-ceous nanomaterials can enhance the conduc-tivity of electrodes as well as advance their electrochemical activity to overcome the stress induced during continuous charge–dis-charge cycling, and this is an effective way to harness their excellent reversible theoretical capacity. As an anode material for superca-pacitor application, α-Fe_2O_3/rGO/g-C_3N_4 composite exhibited specific capacitance of the samples is 650 Fg^{-1} at 1Ag^{-1} current den-sities for α-Fe_2O_3/rGO/g-C_3N_4 which is higher than that of binary α-Fe_2O_3/rGO (510 Fg^{-1} at 1Ag^{-1}) and pure α-Fe_2O_3 (450 Fg^{-1} at 1Ag^{-1}). The synergistic effect between α-Fe_2O_3/rGO/g-C_3N_4 nanocomposites was well studied through various characterization techniques like XRD, FTIR, FE-SEM, HRTEM, UV–vis DRS, PL, XPS. In addition, the α-Fe_2O_3/rGO/g-C_3N_4 nanocomposite exhibits excellent ternary nanostructures for supercapacitor application.

P-76

Enhanced photocatalytic performance of natural clay supported Samarium tungstate nanocomposite

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In the present study, we report the synthesis of samarium tungstate supported on natural clay [$CSm_2(WO_4)_3$] using hydrothermal method. The synthesized [$CSm_2(WO_4)_3$] was extensively characterized by powder X-ray diffraction (XRD), field emission transmission electron microscopy (FE-SEM), energy dispersive X-ray spectroscopy (EDX), Solid UV-Visible spectroscopy and photo-luminance (PL) spectroscopy. The XRD pattern reveals the crystalline size and phase of the nanoparticles and the formation of spherical morphology was confirmed by HR-TEM images. The natural clay support was confirmed by EDX. The band gap energy of

$Sm_2(WO_4)_3$(4 eV) was reduced by natural clay supported [$CSm_2(WO_4)_3$]as 2.6 eV. The photocatalytic activity of $CSm_2(WO_4)_3$ nano-composite was examined by the degradation of oflaxacin (OFLC) and ibuprofen (IBP) by visible light irradiation. Almost complete degradation of oflaxacin and ibuprofen oc-curred at 110 and 80 minutes respectively. $CSm_2(WO_4)_3$ was stable and recyclable up to 5 cycles. This catalyst will be an efficient photocatalyst for the removal of toxic chemi-cals in the environment.

P-77

A study on microbial extract reduced silver nanoparticles assisted biological degradation of pre-treated high-density polyethylene

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The accumulation of plastic wastes in the soil and the available strategies for the management of plastic wastes have accompanied with various environmental pollutions. Nano-materials have been used in the solving of various environmental problems. Thus, the present study is planned to investigate whether the exposure of silver nanoparticles synthesized from the microbial consortium of plastics dumping area to promote the biodegradation of the pre-treated high-density polyethylene (HDPE). First, the study has optimized the synthesis of silver nanoparticles (AgNPs) based on their color intensity, UV absorption and the level of reactive oxygen species (ROS). The optimized AgNPs were extensively characterized through the advanced microscopic (SEM & TEM) and spectral techniques (DLS & FT-IR). The AgNPs were depicted highly intense brown color, characteristic UV absorption, higher levels of ROS, spherical morphology, hydrodynamic size of 1-4.9nm and zeta potential of -200mV. The involvement of functional groups for the reduction of Ag+ to Ag0 and stabilization of AgNPs also identified. Second, the high-density polyethylene films are pre-treated with concentrated nitric acid for 15days, which showed the surface erosion and deformation of the hydrocarbon chain under the micro-scopic and spectral analyses. Then, the pre-treated HDPE films are treated with AgNPs for 15 days and further subjected to the expo-sure of UV light for 5 h. Finally, HDPE films are subjected to biological degradation through the soil burring for 35 days. The sur-face erosion and breaking of hydrocarbon backbone and weight reduction of the studied HDPE were most remarkable in each of the treatment stages. This study suggests that AgNPs-ROS assisted chain breaking and ox-idation reactions could be the reasons for ex-tensive surface modification and degradation of HDPE. Our further study will confirm the contribution of soil microorganism(s) in the biodegradation of HDPE.

P-78

Biological removal of cadmium from soil by phytoremediation and its impact on growth parameters, photosynthetic pigments and antioxidant enzyme in *Brassica nigra*- the indian mus-tard

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Land and water are the most important natural resources for the sustainability of mankind. However due to the industrialization and urbanization, these resources are rapidly contaminated and

depleted. Heavy metal contamination is one such major threat.

Phytoremediation is a novel strategy that is being increasingly used in environmental clean up. The scope of this study is to use *Brassica nigra* (the Indian mustard) for removal of cadmium, a common heavy metal found in contaminated soil. The selected plant was grown in soils contaminated with known amount of cadmium. Its growth was monitored over a period of 28 days. The levels of cadmium in the soil and plant parts were assessed periodically. The extent of stress caused to the plant was measured by quantifying its antioxidant enzymes.

The level of cadmium in the soil is significantly lowered while the plant parts, viz, root and leaves show accumulation of cadmium. There is also an increase in the activity of antioxidant enzymes in the test plant. The levels of carbohydrates, protein, chlorophyll and carotenoids were also found to be higher than the control plant. *Brassica nigra* is a good bio-accumulator.

P-79

A review on various methods used for recognition of urine particles using dig-ital microscopic images of urine sedi-ments

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Urine sediment examination is important for any patient with renal disease. Urinalysis may be physical, chemical or microscopic examinations. Microscopic examination determines the parameters such as Red Blood Cells (RBC), White Blood Cells (WBC), Epithelial Cells, Crystals, Bacteria, and Casts. Results from this test identify various kidney-related diseases such as Hematuria, Kidney Stones, etc. This literature compares various automated methods used for urinalysis. The traditional method for microscopic examination is performed manually on sediment from a centrifuged urine sample. It is a time-consuming process and also there is a possibility of manual errors. This work describes the classification of microscopic images of urine sedi-ments by conventional automated micro-scopic techniques and by using different types of convolutional neural networks (CNN). The problem with the conventional automated models is that the segmentation and feature extraction to be carefully de-signed. The characteristics of microscopic urine images make it a formidable task. The convolutional neural network classifies the images without feature extraction and seg-mentation. Various convolutional neural net-works proposed in the literature are different types of RCNN, SSD and its variants and Le-Net-5 neural network.

P-80

Cerium oxide nanoclusters application in ROS nanobiosensing

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Oxidative stress is a condition where our body is exposed to a chronic low dose of ox-idants which escape the antioxidant system of our body. Oxidants (ROS and RNS) are pro-duced both endogenously due to metabolic activities as well as exogenously due to expo-sure to pollutants as well as radiations etc. in our body. Oxidative stress is responsible for many diseases and plays an important role in

the etiology of cancer. Nano ceria has a dual property of radical scavenging as well as acting as a prooxidant depending on its trivalent and tetravalent state. In the present study, we have synthesized cerium oxide nanoclusters (CeO_2-NCs), and characterized them using different photo physical tools. The ceria nanoclusters exhibited high fluorescence property which was utilized for the detection of ROS. As a source of ROS, we have used hydrogen peroxide and as a radical scavenger ascorbic acid is being used. Our results showed that with the increase in concentra-tion of H_2O_2 the fluorescence intensity in-creased and with increase in ascorbic acid the fluorescence intensity decreased. The change in fluorescence due to H_2O_2 as well as Ascor-bic acid was linear. Thus, it can be proposed that CeO_2-NCs can be used to detect ROS. In future ROS in biological sample needs to be explored

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Synthesis and characterization of iron oxide nanoparticles

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Iron oxide nanoparticles possess better colloidal stability, optical, semiconductor properties, high surface-to-volume ratio, enhanced catalytic effect, biocompatibility, low toxicity and high magnetic moments. These salient features make them an excellent candidate for the biomedical and technological applications. The three most common form of iron oxide in nature are magnetite, hematite and maghemite. The crystal structure of the iron oxide exist as close packed planes of oxygen anions with iron cations in octahedral or tetrahedral interstitial sites. Iron oxide nanoparticles have widespread biomedical applications such as targeted magnetic drug delivery, magnetic resonance imaging, hyperthermia, biosensors, and theranostics. They have potential technological applications such as production of inorganic pigments, magnetic storage media, gas sensors electronic and optical devices, information storage, aerospace and wastewater treatment adsorbents. It is essential to investigate the magnetic properties of the iron oxide nanoparticles in detail as they play a major role in both the biomedical and technological applications.

In the present work, we have prepared iron oxide nanoparticles using hydrothermal method. Iron (III) chloride has been used as precursor and sodium hydroxide has been used as reducing agent. The formation of iron oxide nanoparticles has been confirmed by scanning electron microscopy measurements. We are going to investigate the magnetic properties of the prepared iron oxide nano-particles using vibrating sample magnetome-ter measurements.

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Biodegradable products using sawdust

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Saw dust is a by-product or waste product of woodworking operations such as sawing, milling, planing, routing, drilling and sanding etc. Usage of saw dust to make degradable products are an efficient way to make use of this waste product. It is also relatively abundant and an inexpensive material.

Saw dust is composed of chemicals such as carbon, hydrogen, nitrogen, lignin and holo-cellulose. In order to make use of sawdust to produce biodegradable articles, it must be made into a paste from which the required ar-ticles can be casted using moulds.

Generally, saw dust does not possess cohe-sive properties. Hence it was mixed with suit-able binding material which increases the binding property of saw dust and enhances the flexibility of the material. This mixture was spread in moulds, cooled at room tem-perature and later were taken out.

Since saw dust is obtained naturally from trees, it is a non-pollutant. It is biodegradable and thus it is environmentally sustainable. It can be used to replace plastic products. Using saw dust, also helps in managing waste since saw dust itself is a waste product of the timber industries. Thus, takinginto account the over-all physical, mechanical and environmental properties, saw dust can also be used in the production of commercially available biode-gradable products.

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Bioluminescent plants as a sustainable energy source

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Energy production and conservation is one of the major issues of the modern world. The current ways of generating electricity in-volves laborious extraction, purification and usage of fossil fuels. However, these sources are non-renewable and are also one of the ma-jor causes of environmental pollution. To ad-dress this crisis in a sustainable and eco-friendly way, we aim to create biolumines-cent trees using Genetic Engineering. The phenomenon of Bioluminescence works when Luciferin, a protein reacts with Oxygen in the presence of Luciferase enzyme and Co-enzyme A to give Oxyluciferin. The energy liberated from this reaction is emitted as light. The method involves genetically engineering the plant to make it express the luciferin-en-coding gene obtained from the sources like firefly and jellyfish and thereby emit light. Our target is to perform one treatment when the plant is a seedling or a mature plant, and have it last for the lifetime of the plant. Our work opens up the portal to streetlights that are nothing but treated trees, traffic signals and to indirect lighting around homes. The idea of this project is to create Glow-in-the-Dark Trees using the concept of Biolumines-cence, which could replace the streetlights. This is an environment-friendly, pollution-free method to conserve electricity. This method adopts the readily-available, natural phenomenon (Bioluminescence) to solve practical problems of energy production in an eco-friendly manner. Also, the toxic by-prod-ucts and wastes are not generated in this method. Since this method would require us to depend on plants for energy as well, it would promote floral growth and conserva-tion.

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Development and characterization of chitosan-based transdermal patch of Aceclofenac sodium

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The transdermal patch system is an alternative to invasive injections. Chitosan has gained attention in the pharmaceutical industry for its significant biodegradability, biocompatibility, and non-antigenicity

property (1). These behaviors are beneficial for the development of transdermal drug delivery systems (2). Aceclofenac is a nonsteroidal anti-inflammatory drug used extensively in the treatment of rheumatoid arthritis, osteoarthritis, and ankylosing spondylitis. The short biological half-life (<4 h) and dosing frequency of more than one time a day make it an ideal candidate for modified release formulation.

The purpose of this research was to develop a matrix-type transdermal drug delivery system using natural polymer chitosan. The acrylic acid-based adhesive technique was used to develop the patch system. Aceclofenac sodium was used as the model drug for this present study. In this context, the developed transdermal films were characterized for thickness, weight variation, drug content, flatness, folding endurance and moisture content. Further, the adhesiveness of the transdermal films prepared with chitosan gels were also assessed. All prepared formulations indicated good physical stability. In-vitro permeation studies of formulations were performed by using Franz diffusion cells. It is shown that drug release follows zero-order and the mechanism of release is a diffusion from the polymer. The prepared transdermal patch system of Aceclofenac sodium using Chitosan had shown good promising results for sustained release matrix transdermal patch formulation.

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Light Assisted Killing of Cancer Cells by a Photosensitizer Protein

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Demand to treat cancer is overwhelming day by day as the diversity and mortality rate of cancer is on high inflation, as per WHO reports 2018 there are 18.1 million newly identified cancer cases with 9.6 million deaths worldwide. Even though there are many treatment methods available, major drawback is the requirement of specific medication for effective remedy for distinct types of cancer. In this upraised field of cancer research, we focus on genetically encoded photosensitizer proteins utilization for a targeted therapy. Photosensitizers proteins are basically chromophores that generate reactive oxygen species upon light irradiation. Due to the toxic reactive nature of this photosensitizer protein they are biologically utilized for inactivation of selected proteins in chromophore-assisted light inactivation (CALI) technique and the light-induced cell killing in Photodynamic therapy (PDT). Major limitation in this PDT cancer treatment is the targeted delivery of these photosensitizers to the specific cancer cell. To over-come this drawback, we have engineered photosensitizer protein variants that are capable of entering cancer cells without using any specialized reagents. This photosensitizer protein produces toxic free radicals upon exposure to light. We demonstrate that the engineered photosensitizer protein variants are able to enter and kill cancer cells readily upon exposure to green light. We engineered and purified several such protein variants using E. coli as an expression host. Using HeLa cells, we observed that more than 90% cells show internalization of the recombinant protein within 4 hours of incubation. Post internalization these cells were killed within 10 minutes of exposure to the green light. After establishing the proof of concept, now we have designed several protein variants which will be evaluated to test internalization and killing of specific cancer cell types.

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Identifying common pathways and checkpoints in neurodegenerative diseases by enrichment analysis

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Neurological disorders as one of the greatest threats to public health. There are several gaps in understanding the many issues related to neurological disorders. It affects the central and peripheral nervous system and include disorder like epilepsy, Alzheimer and other dementias, multiple sclerosis, Parkinson's disease and prion disease. By WHO statistics, around 5 million people die due to stroke per annum. More than 50 million people have epilepsy. Around 7 million new cases of dementias are treated every year. Of these dementia cases, 60-70% turns out to be Alzheimer's. Certain microbial infections and immune responses may also cause neurological symptoms. Hence, the neurological disorders are rather difficult to distinguish due to their similar symptoms and presentations in clinical cases. Complexity of the disease pathways and highly similar causative genes make the diagnostics more complex.

The project focuses on identifying the common pathways and genes involved in neurodegenerative diseases. This work focuses on differentiating the effects by biological functions and identifying the shared pathway from which the effect deviates. We processed gene data of the selected disease and per-formed a meta-analysis to obtain true hetero-geneous genes with its functional annota-tions. CD2BP2, MT2A, HVCN1, CHRM1, IQGAP1, GABARAP, EDF1, IMP3, FXYD7, FAM161B, CDK5, ERCC1, PTPN13, CYC1, PHTF2, NSUN6. These are the genes found common across the gene datasets from different diseases. Further, the pathway enrichment analysis will be done to identify outliers and common pathways to validate the common genes as biomarkers for different neurodegenerative diseases leading to enhanced diagnostics.