SVKM'S NMIMS Deemed to be UNIVERSITY

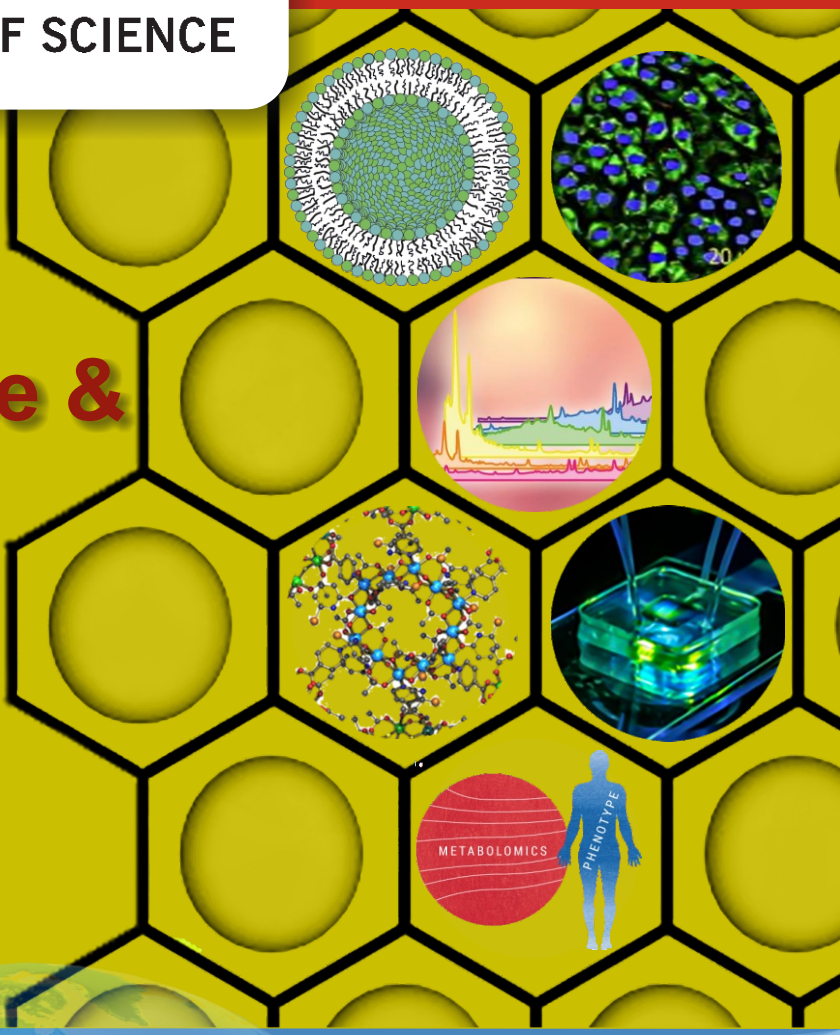
SUNANDAN DIVATIA SCHOOL OF SCIENCE

International Conference on

# Advances in Materials Science & Applied Biology (AMSAB-2019)

8th–10th January 2019

Mukesh Patel Auditorium
SVKM's NMIMS (Deemed-to-be University)
Mumbai, India




# Abstract Book

Organized by

Sunandan Divatia School of Science
NMIMS (Deemed to be University)

International Conference on

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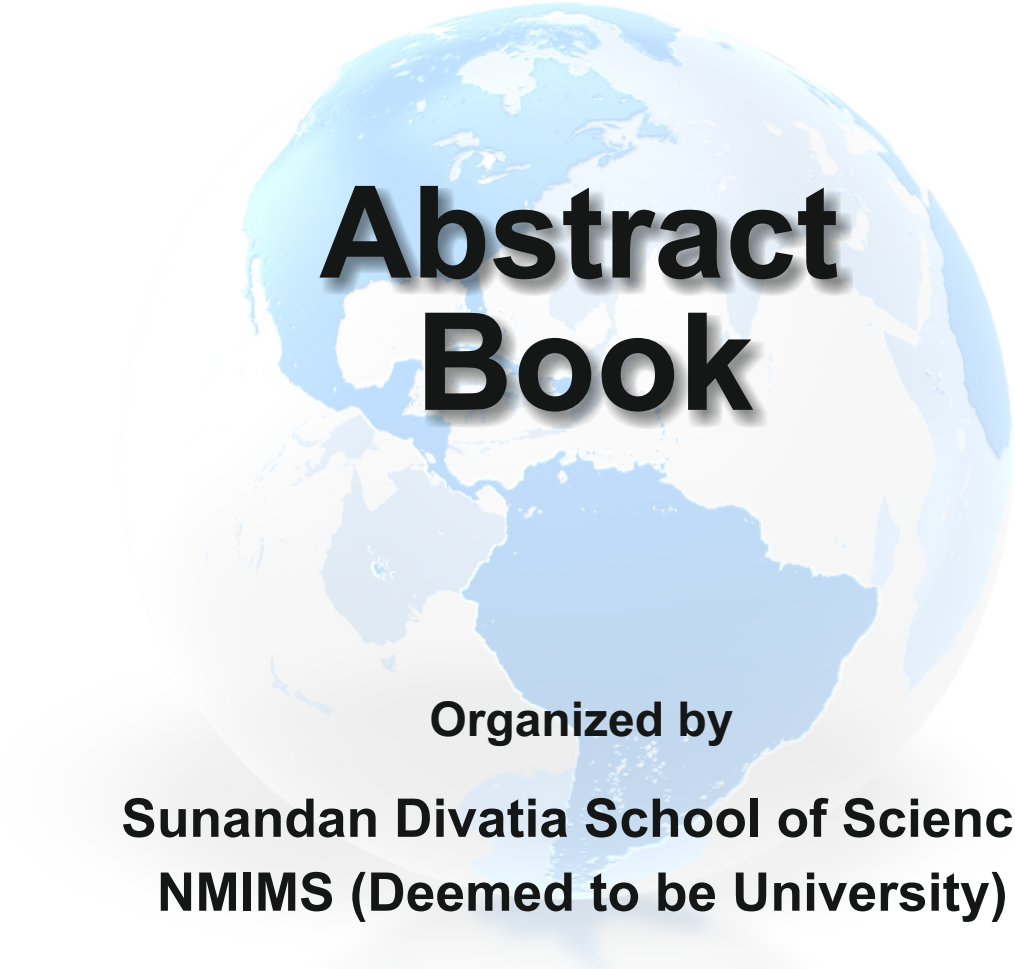

# Abstract Book

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# MESSAGE FROM VICE-CHANCELLOR

SVKM's NMIMS (Deemed-to-be University) is one of the leading top private University for higher studies in India. The Sunandan Divatia School of Science (SDSOS) is one of the schools of the prestigious SVKM'S NMIMS which serves as a Center of excellence that performs advanced research in Applied Science, promotes interdisciplinary research and provides quality education to students.

I welcome all the participants to the International conference on Advances in Material Science and Applied Biology 2019. I congratulate the academic and non-academic staff members, as well as students of Sunandan Divatia School of Science who have worked collectively in organizing the conference.

I believe that AMSAB 2019 would serve as an excellent platform for leading international and national scientists to share advancements in scientific research and opening up the prospects of collaboration. Such international level events facilitate knowledge based innovation and mark the advancement in science and technology. Young minds in the field of Science and technology will also greatly benefit by learning cutting-edge scientific developments and cultivate better learning for the benefit of health and well-being. This conference will provide tremendous exposure and opportunities to all participants and contribute immensely to the betterment of the society.

I convey my best wishes to all the participants and organizers of the conference in all your future endeavors.

## MESSAGE FROM CONFERENCE CHAIR

It gives me immense pleasure to invite all renowned scientists, academicians, as well as researchers from all over the globe to attend the International conference on Advances in Material Science and Applied Biology 2019 organized by SVKM's NMIMS Sunandan Divatia School of Science. This three-day conference is designed to highlight latest developments in fields of nanoscience, drug delivery, material science as well as several aspects of applied biology like bio and chemi-informatics and tissue engineering.

The conference aims to bring together experts, scholars and researchers from different parts of the globe on a common platform to discuss the advances and challenges in the above areas. It seeks to promote top level research and to globalize quality research thus making presentations and discussions more internationally competitive and focusing attention on the recent outstanding achievements in the field of material sciences and applied biology and future trends and needs.

I am looking forward to an excellent conference with great scientists discussing various aspects of inter disciplinary research in related areas and participants getting opportunity to listen to distinguished experts. Further the conference will stimulate development of novel collaborations towards performing cutting edge research and open novel fields of research for budding scientific minds. The young researchers would also gain from attending and networking with scientists in the field.

I wish the conference a great success and look forward to a stimulating scientific debate, develop novel collaborations and benefit young scientific minds.

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# THEMES OF THE CONFERENCE

**Nano-drug Delivery and Therapeutics**

- Novel drug delivery systems
- Synthesis of nanomaterials
- Drug targeting and design
- Smart drug delivery systems
- Nanotoxicity
- Cancer and nanotechnology
- Advanced functional materials
- Nano medicine for Infectious and Non-infectious diseases
- Nano medicine in theranostics
- Nano carriers
- Major challenges in drug delivery
- Photodynamic therapy

**Bio- and Chemi-Informatics**

- NextGen sequencing
- Genomics
- Chemical library screening
- Drug design and docking
- Pharmacogenomics
- Application in diseases

**Biomaterials and Tissue Engineering**

- Biomaterials and mechanobiology
- Biomaterials for stem cell propagation
- Tissue engineering (bone, cartilage, skin etc.)
- Nano and micro-fabricated hydrogels
- Tissue engineering for drug discovery
- Tissue engineering and regenerative medicine
- Challenges in biomaterials for tissue engineering

**Applications of Material Chemistry**

- Energy and environment
- Devices and sensors
- Nanocatalyst for solar fuel
- Supercapacitor and battery
- Nano biosensors
- Electrochemistry
- 2-D and 3-D imaging
- Nanoporous material
- Fuel cells
- Bio fuels

**Applied Spectroscopy**

- Mass spectroscopy
- EPR
- Fluorescence spectroscopy
- X-ray photon spectroscopy
- Raman spectroscopy
- Circular dichrosim
- Atomic absorption and emission spectroscopy
- ICP-AES
- Mossbauer spectroscopy
- Electrochemical impedance spectroscopy

**Metabolomics Research**

- Metabolic engineering
- Metabolic profiling and finger printing
- Metabolite target analysis
- Systems biology
- Tools and techniques in metabolomics research
- Challenges in metabolomic research

# TECHNICAL SESSIONS

## AMSAB 2019 SCHEDULE Day 1 (08-01-2019; Tuesday)

| Time (IST) | Schedule | Chair Persons |
|---|---|---|
| 8:30 - 9:30 | Registration and Breakfast | |
| 9:30 - 10:00 | Welcome and Inauguration | |
| 10:00 - 11:00 | **Plenary talk: Padma Vibhushan Professor MAN MOHAN SHARMA** (Former Director, Institute of Chemical Technology Mumbai, India) | **Dr. Anant Jhaveri** |
| 11:15-12:00 | **Keynote 1: HEINRICH LANG** (Technical University of Chemnitz, Germany)<br>Title: From: Small Tailor-made Molecules To: New Materials | **Dr. Sagar Mitra** IIT- Bombay & **Dr. Haridas Pal,** BARC |
| 12:00 -12:30 | **Invited Speaker 1: VIVEK POLSHETTIWAR** (Tata Institute of Fundamental Research, Mumbai, India)<br>Title: Advanced Nanomaterials for Harvesting Solar Energy, Catalysis and $CO_2$ Capture | |
| 12:30 - 13:10 | **Oral Talk 1: SAHADEV SHANKARAPPA** (Amrita Institute of Medical Science, Kochi, India)<br>Title: Peripheral nerve fibres within thick-skin as a route for nanoparticle delivery<br>**Oral Talk 2: CHRISTINA NUTSCHEL** (Heinrich Heine University Düsseldorf, Germany)<br>Title: Large-scale analysis of protein thermostability and detergent tolerance | |
| 13:10 -14:00 | Lunch | |
| 14:00 - 14:45 | **Keynote 2: EHUD GAZIT** (Tel Aviv University, Israel)<br>Title: Peptide and Metabolite Materials: A Reductionist Approach | **Dr. Holger Gohlke** Heinrich Heine University Düsseldorf & **Dr. Sudeshna Chandra,** NMIMS |
| 14:45 - 15:15 | **Invited Speaker 2: VANDANA PATRAVALE** (Institute of Chemical Technology, Mumbai, India)<br>Title: Functionalized Nanosystems as Trojan horses for Superior Therapeutics | |
| 15:15 - 15:45 | **Invited Speaker 3: JAYAKUMAR RANGASAMY** (Amrita Institute of Medical Sciences & Research Centre, Kochi, India)<br>Title: Multiple Applications of Injectable Hydrogels | |
| 15:45 - 16:00 | Tea and Networking | |
| 16:00 - 16:30 | **Invited Speaker 4: GANESH VISHWANATHAN** (Indian Institute of Technology Bombay, Mumbai, India)<br>Title: Topological and functional analysis of a comprehensive TNFα signaling network | **Dr. Evans Coutinho** BCP & **Dr. Heinrich Lang** TU Chemnitz |
| 16:30 - 17:30 | **Oral Talk 3: PRATAP KOLLU** (Center for Advanced Studies in Electronic Science and Technology, School of Physics, University of Hyderabad, Hyderabad, India)<br>Title: Smart magnetic sensors and Development of a magnetoresistive biosensor for the detection of biomolecules<br>**Oral Talk 4: ROHAN SHAH** (Department of Chemistry and Biotechnology, Swinburne University of Technology, Victoria, Australia)<br>Title: Small angle scattering studies of solid lipid nanoparticles in solution<br>**Oral Talk 5: PRADIP KUMAR** (Department of Physics, Central University of Rajasthan, Ajmer, India)<br>Title: Graphene-structured materials for highly active and durable oxygen reduction electrocatalyst | |
| 17:30 - 18:30 | **Poster Session** | |
| 18:30 - 19:30 | Cultural Program | |
| 19:30 | Conference dinner | |

# AMSAB 2019 SCHEDULE Day 2 (09-01-2019; Wednesday)

| Time (IST) | Schedule | Chair Persons |
|---|---|---|
| 8:30 - 9:30 | Breakfast | |
| 9:30 - 10:15 | **Keynote 3: K V VENKATESH** (Indian Institute of Technology Bombay, Mumbai, India)<br>Title: Systems Engineering Perspective of Human Metabolism through a Multiscale Model for Disease Analysis : A Cell to Human Framework | **Dr. Shubhada Chiplunkar** ACTREC & **Dr. Padma Devarajan** ICT |
| 10:15 - 10:45 | **Invited Speaker 5: KAUSHIK CHATTERJEE** (Indian Institute of Science, Bengaluru, India)<br>Title: Biomaterials for Engineering Organotypic Culture Models for Breast Cancer and Cardiac Diseases | |
| 10:45 -11:15 | **Invited Speaker 6: SHAILENDRA GIRI** (Henry Ford Health System, USA)<br>Title: Blood-based untargeted metabolomics in Relapsing-Remitting Multiple Sclerosis revealed testable therapeutic target. | |
| 11:15-11:30 | Tea and Networking | |
| 11:30-12:30 | **Oral Talk 6: DHIRAJ BHATIA** (Department of Biological Engineering, IIT Gandhinagar, Gandhinagar, India)<br>Title: DNA Based Emerging Technologies for Biological Applications<br>**Oral Talk 7: PRIYAL CHIKHALIWALA** (Sunandan Divatia School of Science, NMIMS (Deemed-to-be University), Mumbai, India)<br>Title: Development of electrochemical nano-immunosensor for early detection of hepatocellular carcinoma<br>**Oral Talk 8: MANASHJIT GOGOI** (Department of Biomedical Engineering, North Eastern Hill University, Shillong, India)<br>Title: Therapeutic evaluation of magnetic liposomes engineered for self-controlled hyperthermia and chemotherapy | **Dr. Munira Momin** BNCP & **Dr. Purvi Bhatt** NMIMS |
| 12:30 -13:00 | **Invited Speaker 7: PRAKRITI TAYALIA** (Indian Institute of Technology Bombay, Mumbai, India)<br>Title: Porous synthetic matrices as platforms for immunotherapy and cancer studies | |
| 13:00 -14:00 | Lunch and Poster Session | |
| 14:00 - 14:45 | **Keynote 4: TANEMURA MASAKI** (Nagoya Institute of Technology, Japan)<br>Title: Catalytic Activity on Low Temperature Graphene Growth based on Dynamic TEM Observations | **Dr. Shailendra Giri** Henry Ford & **Dr. Gurudas Mane** NMIMS |
| 14:45 - 15:15 | **Invited Speaker 8: ABHIJIT DE** (Advanced Centre for Treatment, Research and Education in Cancer, Mumbai, India)<br>Title: Avenues of *in vivo* Multimodality Imaging during Development of Cancer Nanotherapeutics | |
| 15:15 - 16:15 | **Oral Talk 9: DEEPALI KADUSKAR** (SVKM's NMIMS, SPP SPTM, Mumbai, India)<br>Title: Preparation and evaluation of bioactive glass scaffolds containing levonorgestrel by 3D printing approach for bone tissue regeneration.<br>**Oral Talk 10: MANEKA HOONJAN** (Sunandan Divatia School of Science, NMIMS (Deemed-to-be University), Mumbai, India)<br>Title: Folic acid conjugated arsenic trioxide nanoparticles for improved drug delivery<br>**Oral Talk 11: TARU DUBE** (Institute of Nano Science and Technology, Mohali, India)<br>Title: Self-assembled levodopa tubes mediated synthesis of Au microroses as SERS probes in C6 glioma cells | |
| 16:15 - 16:30 | Tea and Networking | |
| 16:30 - 17:00 | **Invited Speaker 9: ASHOK RAICHUR** (Indian Institute of Science, Bengaluru, India)<br>Title: To be announced | |
| 17:00 - 17:30 | **Invited Speaker 10: SHILPA N SAWANT** (Bhabha Atomic Research Centre, Mumbai, India)<br>Title: Electrochemical Biosensors for Metabolite Detection | |
| 17:30 | Concluding Remarks | |

# AMSAB 2019 SCHEDULE Day 3 (10-01-2019; Thursday)

| Time (IST) | Schedule | Chair Persons |
|---|---|---|
| 8:30 - 9:30 | Breakfast | |
| 9:30 - 10:15 | **Keynote 5: TAPAS SEN** (University of Central Lancashire, UK)<br>Title: Functional Nanomaterials in CleanTech and Medicine: An overview of our past and on-going UKIERI projects | **Dr. Vandana Patravale** ICT & **Dr. Brijesh S.** NMIMS |
| 10:15 - 10:45 | **Invited Speaker 11: VIVEK TANAVDE** (Ahmedabad University, India)<br>Title: miRNA regulation of stem cell differentiation: Do miRNA networks regulate signalling networks in differentiating Mesenchymal Stromal Cells? | |
| 10:45 -11:15 | **Invited Speaker 12: GITANJALI YADAV** (National Institute of Plant Genome Research, New Delhi, India)<br>Title: Identification and Analysis of KIX domains and their Interacting partner Transactivation Domains (TAD) during Transcription | |
| 11:15-11:30 | Tea | |
| 11:30-12:10 | **Oral Talk 12: AYAN MAITY** (Department of Chemical Sciences, TIFR, Mumbai, India)<br>Title: Highly Monodisperse Dendritic Fibrous Nanosilica: Scalable Synthesis Quantified by E-Factor and Applications in Lasing by Self-Assembled Photonic Crystals<br>**Oral Talk 13: VRUSHALI S. JOSHI** (Sunandan Divatia School of Science, SVKM's NMIMS, Mumbai, India)<br>Title: Real-Time Metabolic Interactions between Two Bacterial Species Using a Carbon-Based pH and Peroxide Microsensors as a Scanning Electrochemical Microscopy Probes | **Dr. Shilpa Sawant** BARC & **Dr. Nancy Pandita** |
| 12:10 -12:40 | **Invited Speaker 13: MUSTHAFA MUHAMMED** (Indian Institute of Science Education and Research, Pune, India)<br>Title: Realization of Hydrogen Economy with Electrochemical Energy Devices | |
| 12:40 -13:40 | Lunch | |
| 13:40 - 14:25 | **Keynote 6: HOLGER GOHLKE** (Heinrich Heine University Düsseldorf, Germany, India)<br>Title: Functional selectivity and basal activity of G-protein coupled receptors deduced from network rigidity | **Dr. Dhananjaya Saranath** CPAA & **Dr. Aparna Khanna** NMIMS |
| 14:25 - 14:55 | **Invited Speaker 14: SHAILZA SINGH** (National Centre for Cell Science, Pune, India)<br>Title: Systems driven Synthetic bio therapeutics device in Leishmaniasis | |
| 14:55 - 15:25 | **Invited Speaker 15: PRAVEEN KUMAR VEMULA** (InStem, Bengaluru, India)<br>Title: Disease-responsive biomaterials: A novel concept for the treatment of autoimmune and inflammatory diseases | |
| 15:25 - 15:40 | Tea | |
| 15:40 - 16:10 | **Invited Speaker 16: ROHIT SRIVASTAVA** (Indian Institute of Technology Bombay, Mumbai, India)<br>Title: Affordable Healthcare Technologies | |
| 16:10 - 16:50 | **Oral Talk 14: K. C. BARICK** (Chemistry Division, Bhabha Atomic Research Centre, Mumbai, India)<br>Title: Interfacial modification of inorganic nanoparticles for drug delivery applications<br>**Oral Talk 15: NEETHU C. D.** (IISER Pune, Pune, India)<br>Title: A Rechargeable Hydrogen Battery | |
| 16:50- 17:15 | Valedictory and Conclusion followed by Tea | |

# INDEX

## PLENARY TALK

### About the Plenary Speaker

Padma Vibhushan Professor Man Mohan Sharma is a distinguished scientist in the field of Chemical Engineering. With immense pleasure, we welcome him as a plenary speaker for our conference.

Prof. Sharma has made several contributions to chemical engineering science and technology. His studies on Bronsted based catalysis in $CO_2$ hydration (published in the Transactions of Faraday Society) and subsequently kinetics of COS absorption in aqueous amines and alkanolamines brought out linear free energy relationship between $CO_2$ and COS absorption in solutions of amines and alkanolamines. His research has added extensively on the role of microphases in multiple reactions which he pioneered. He was appointed as an independent Editor of Chemical Engineering Science at a young age. He taught different subjects in chemical engineering and encouraged his doctoral students, from the very beginning, to publish independently their work in renowned journals.

Prof. Sharma did his BE in Chemical Engineering from the University of Bombay (1958), and his PhD from the University of Cambridge (1964). He was Professor of Chemical Engineering at UDCT (University of Bombay, Department of Chemical Technology, Mumbai) and retired as the Director of UDCT.

Prof. Sharma has countless awards to his credit. To mention a few; he was awarded the Padma Bhushan (1987) and the Padma Vibhushan (2001) by the President of India. He has also been awarded the Leverhulme Medal of the Royal Society, the S.S. Bhatnagar Prize in Engineering Sciences (1973), FICCI Award (1981), the Vishwakarma medal of the Indian National Science Academy (1985), G.M. Modi Award (1991), Meghnad Saha Medal (1994), and an honorary Doctor of Science degree from Indian Institute of Technology, Delhi (2001).

# KEYNOTE TALKS

**KN 01**

## From: Small Tailor-made Molecules To: New Materials

HEINRICH LANG
Technische Universität Chemnitz, Faculty of Natural Sciences, Institute of Chemistry, Inorganic Chemistry, D-09107 Chemnitz (Germany)
heinrich.lang@chemie.tu-chemnitz.de

Within this presentation a brief overview of our group's topics in the field of material sciences will be given.

The main focus of the talk will be directed to the use of novel organometallic and metal-organic compounds based on different transition metals (for example, Cu, Ru and Co) as precursor molecules in gas-phase (Chemical Vapour Deposition, Atomic Layer Deposition) and spray-coating deposition technologies for the generation of thin conformal metal films and patterns.

Also the use of combustion-CVD and inkjet printing of metal-organic inks to produce conductive and semi-conductive layers on flexible substrates will be reported.

A straightforward synthetic methodology for the generation and stabilization of conductive, semi-conductive and magnetic metal as well as metal oxide nanoparticles by using single-source coordination complexes, such as $L_nM(O_2CCH_2(OCH_2CH_2)_2OMe)_m$ ($L_nM$ = Ag, $Cu(PR_3)_2$, $Au(PR_3)$, $Ru(PR_3)_2(CO)_2$, $Pd(PR_3)_2$, $Pt(PR_3)_2$, Rh, Mn, Co, Ni, Fe, …; m = 1, 2, 3) as precursors will be envisaged.

Finally, the possibility to apply metal nanoparticles for joining materials at low temperature using the soldering process will be reported, as well as laser ablation for the generation of metallic structures from metal-organic complexes.

**KN 02**

# Peptide and Metabolite Materials: A Reductionist Approach

EHUD GAZIT FRSC OSSI
Department of Molecular Microbiology and Biotechnology, Department of Materials Science and Engineering, Tel Aviv University, Tel Aviv 69978, Israel
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The formation of ordered nanostructures, with unique physical properties, by the molecular self-assembly of proteins and peptides represents one of the principal directions in nanotechnology.[1] Indeed, polyamides provide superior features as materials with diverse physical properties. A reductionist approach allowed the identification of extremely short peptide sequences, as short as dipeptides, which could form well-ordered amyloid-like β-sheet-rich assemblies comparable to supramolecular structures made of much larger proteins. Some of the peptide assemblies show remarkable mechanical, optical, and electrical characteristics.[2] Another direction of reductionism utilized a natural noncoded amino acid, α-aminoisobutryic acid, to form short superhelical assemblies. The use of this exceptional helix inducer motif allowed the fabrication of single heptad repeats used in various biointerfaces, including their use as surfactants and DNA-binding agents. Two additional directions of the reductionist approach include the use of peptide nucleic acids (PNAs) and co-assembly techniques.[3,4] Finally, our reductionist approach also led to the development of metabolite (amino acid and nucleobase based materials).[5]

**References**

1. Gazit, E., Reductionist approach in peptide-based nanotechnology. *Annu. Rev. Biochem.* 2018, *87*, 533.
2. Tao, K.; Makam, P.; Aizen, R.; Gazit E. Self-assembling peptide semiconductors. *Science* 2017, *358*, eaam9756.
3. Berger, O.; Adler-Abramovich, L.; Levy-Sakin, M.; Grunwald, A.; Liebes-Peer, Y.; Bachar, M.; Buzhansky. L.; Mossou, E.; Forsyth, V.T.; Schwartz, T.; Ebenstein, Y.; Frolow, F.; Shimon, L.J.; Patolsky, F.; Gazit, E. Light-emitting self-assembled peptide nucleic acids exhibit both stacking interactions and Watson-Crick base pairing. *Nature Nanotechnol.* 2015, *10*, 353.
4. Makam, P.; Gazit, E., Minimalistic peptide supramolecular co-assembly: expanding the conformational space for nanotechnology. *Chem. Soc. Rev.* 2018, *47*, 3406.
5. Aizen, R.; Tao, K.; Rencus-Lazar, S.; Gazit, E.. Functional metabolite assemblies -a review. *J. Nanoparticle Res.* 2018, *20*, 125.

**KN 03**

# Systems Engineering Perspective of Human Metabolism through a Multiscale Model for Disease Analysis: A Cell to Human Framework

K. V. VENKATESH
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Human physiology is an ensemble of various biological processes spanning from intracellular molecular interactions to the whole body phenotypic response. Systems biology endures to decipher these multi-scale biological networks and bridge the link between genotype to phenotype. The structure and dynamic properties of these networks are responsible for controlling and deciding the phenotypic state of a cell. Several cells and various tissues coordinate together to generate an organ level response which further regulates the ultimate physiological state. The overall network embeds a hierarchical regulatory structure, which when unusually perturbed can lead to undesirable physiological state termed as disease. Here, we treat a disease diagnosis problem analogous to a fault diagnosis problem in engineering systems. Accordingly we review the application of engineering methodologies to address human diseases from systems biological perspective. The research work highlights potential networks and modeling approaches used for analyzing human diseases. The application of such analysis is illustrated in the case of diabetes and hypercholesterolemia. We put forth a concept of cell-to- human framework comprising of five modules (data mining, networking, modeling, experimental and validation) for addressing human physiology and diseases based on a paradigm of system level analysis. The work emphasizes on the importance of multi-scale biological networks and subsequent modeling and analysis for drug target identification and designing efficient therapies.

International Conference on
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**KN 04**

# Catalytic Activity on Low Temperature Graphene Growth based on Dynamic TEM Observations

MONA ARABY, SAHAR ELNOBI, SUBASH SHARMA, GOLAP KALITA, MASAKI TANEMURA
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ZAMRI YUSOP
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Graphitized nanocarbon, such as graphene and carbon nanotube (CNT), is one of the hottest materials in nanotechnology and nanomaterials science, thus myriads of applications are expected. The subjects to be solved for realizing those applications include their controllable synthesis, namely, controllability in crystallinity, size, growth position, growth temperature and so on. In order to achieve the growth controllability, understanding of their growth process by its detailed observation in atomic dimension will be indispensable. In this talk, we will deal with a challenge to the graphene growth at temperatures as low as 150-250°C based on the findings in the in situ dynamic transmission electron microscope (TEM) observations of the graphitization process in the solid (liquid) phase reaction [1, 2].

For the in situ TEM observation, 1-dimensional amorphous carbon nanofibers (CNFs) with a metal inclusion were fabricated on an edge of a carbon foil by $Ar^+$ ion irradiation with a simultaneous supply of variety of metals at room temperature [3-6]. This sample preparation method was quite useful for the survey of catalytic property of metals on graphitization, because any kind of metals and semiconductors can be included into CNFs. The samples thus prepared were mounted on a TEM sample holder for the current-voltage (I-V) measurement (two-probe system) without any post treatment, and the transformation process to graphene or to CNT during the electron current flow in the CNF was observed [3-7].

The as fabricated metal-included CNFs were featured by the amorphous CNFs with the inclusion of metal nanoparticles. Depending on the catalytic property of the included metal, CNTs and graphene formed by resistive Joule heating in TEM [3-7]. Among the various catalyst metals survayed, Sn and In were found to be promising for the low temperature growth of graphene, though they have been rarely used for the conventional chemical vapor deposition. Encouraged by this findings, stacked films of Sn/C or In/C were deposited onto $SiO_2$/Si and glass substrates [1, 2]. The thin film samples thus prepared were simply annealed at 150-250°C under vacuum condition. As confirmed by Raman analyses (Fig. 1), the graphene grew even at a temperature as low as 150°C by this simple method [2]. In the talk, possible applications of this low-temperature grown graphene will be also dealt with.

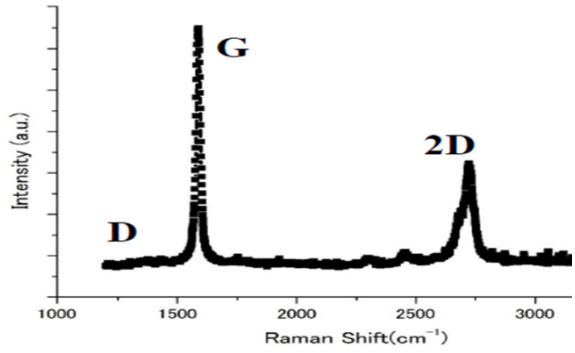


Figure 1: Typical Raman spectrum attained for an In/C film sample vacuum-annealed at 200°C.

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***Keywords***: *graphene growth, low temperature, in situ TEM.*

**KN 05**

# Functional Nanomaterials in CleanTech and Medicine: An overview of our past and on-going UKIERI projects

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The fabrication of functional nanocomposites and their applications *via* surface patterning with chemicals and bio-chemicals has a direct impact in bio-sensing and bio-separation. Surface patterning on nanoparticles in suspension can be a complex process due to the aggregation of the particles and their Brownian motion in the suspension. An overview of group's research on nanomaterials and their applications in the separation of nucleic acids (DNA and RNA) from the biological cells[1,2] will be presented in connection with an industrial collaboration with Q-Bioanalytic, Germany. The possibility of affinity interaction of biomolecules i.e. nucleic acid, protein, antibody, microorganisms etc. through hybrid capture will also be discussed in the context of food quality and hygiene in Bio-sensing[3].

Separation of toxic and microbial contaminants from water and soil using nanotechnology tool will be discussed in the context of recently completed UKIERI project (www.nanowateratuclan.org). Recent development on antimicrobial nanocomposites will be discussed in connection with water-borne microorganism such as E-coli[4-5]. In addition, removal of toxic chemicals and metal ions will also be presented. The talk will also be covered on our on-going UKIERI project (www.uclannanomedicine.net) with Delhi University on functional nanomaterials in Cancer therapy. In this context, some recent work on magnetic nanoparticles in cellular toxicity using magnetic hyperthermia[6,7] will be presented. The proposed talk is the outcome of collaborative work from various academic and industrial organisations around the world and will be focused on both academia and industrial perspective.

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**KN 06**

# Functional selectivity and basal activity of G-protein coupled receptors deduced from network rigidity

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G-protein coupled receptors (GPCR) serve as relays for recognizing signals outside the cell, which are transmitted through the membrane to initiate cellular signaling cascades. Their diverse physiological responses in living cells established GPCRs as important drug targets. Binding of extracellular modulators either induce, inhibit, or alter the activation of GPCRs by stimulating different signaling pathways. However, despite increasing structural information of GPCRs, complemented by intensive computational studies, a detailed knowledge of the signaling mechanisms in GPCRs has remained elusive.

Recently, we introduced a rigorous approximation of vibrational entropy changes upon ligand binding based on analyzing constraint network representations (1) of biomolecular complexes.(2) We also formulated an ensemble- and rigidity theory-based free energy perturbation approach to analyze dynamic allostery.(3) In this work, we apply these methodologies, first, to analyze how different extracellular modulators affect signaling of the GPCRs $\beta_2$ adrenoreceptor (β2AR) and μ-opioid receptor (MOR). Based on altered stability characteristics of the GPCRs, our approaches allow discriminating between agonist, antagonist, and inverse agonist binding and reveal different pathways of connected residues in both β2AR and MOR depending on the type of extracellular modulator. Second, we investigate why the human histamine $H_4$ receptor ($hH_4R$) shows a high degree of constitutive activity in contrast to mouse $H_4R$ ($mH_4R$). By sequence comparison, molecular dynamics simulations, and rigidity analyses, we identify, and experimentally validate, residues in the extracellular loop 2 region of $hH_4R$ that apparently mimic agonist binding and, thus, lead to basal activity.

Overall, our results shed new light on signaling mechanisms in GPCRs at an atomistic level and demonstrate that the rigidity theory-based analysis of dynamic allostery provides a computationally cheap, yet information-rich, way to scrutinize the role of ligands and sequence variations for GPCR signaling.

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# INVITED TALKS

**IT 01**

# Advanced Nanomaterials for Harvesting Solar Energy, Catalysis and $CO_2$ Capture

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Energy and environment are two of our critical societal challenges. The use of hybrid nanomaterials to harvest solar energy as well as capture and convert CO2 seems to be the best way combat climate change. We recently reported the synthesis of a new class of dendritic fibrous nano-silica (DFNS).1-10 Fibrous morphology observed in these nanospheres has not been seen before in silica materials. Uniqueness of DFNS is, its high surface area is by virtue of its fibrous structure instead of pores (unlike MCM-41 and SBA-15 silicas), and hence easily accessible. More than 100 groups worldwide is now using our patented1c DFNS for various applications such as catalysis, solar-energy harvesting, energy storage, self-cleaning antireflective coatings, surface plasmon resonance-based ultrasensitive sensors, CO2 capture, and biomedical applications.1b We showed successful utilization of DFNS for range of important catalytic applications such as metathesis, hydrogenolysis, oxidation, hydrogenation, coupling reactions etc2-8 as well as for CO2 capture.9 We have also developed a new method of fabricating active photocatalysts by TiO2 coating of DFNS.10 In this seminar, I will discuss our results on synthesis and application fibrous nano-silica (DFNS) for confronting with climate change, more specifically for catalysis, solar energy harvesting and CO2 capture.

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**IT 02**

## Functionalized nanosystems as trojan horses for superior therapeutics

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Meticulous and rationalized selection of nano delivery system is crucial for site specific delivery and selective uptake of drugs to the target site. This becomes more challenging while targeting cancer and/ or brain ailments, as the underlying tissue offers additional barriers for drug delivery. In view of this, we have developed battery of functional excipients with dual ability of targeting specific tissue/ cell and self-assembling properties (Patented Technology). For instance, to facilitate superior transfection, endosomal escaping ability and to enhance the intracellular availability of therapeutic actives, we have designed and synthesized a novel amphiphilic, cationic heterolipid. This cationic heterolipid was used to develop novel nanodelivery systems for intratumoral delivery. The specific applications involved fabrication of cationic self-microemulsifying drug delivery system (C-SMEDDS) for drugs and monoguinoplex for gene therapy. The studies revealed not only a significant enhancement in intracellular uptake but also addressed biopharmaceutical issues related to non-site specific drug delivery.

Further, to facilitate transport of drugs across blood brain barrier (BBB) for management of neurodegenerative disorders and infections like cerebral malaria, we have designed and developed multiple lipid bioconjugates with an inherent ability to circumvent BBB via active transport pathway. The micellar and lipid nanocarriers were fabricated using these lipid bioconjugates for drug delivery applications. The studies confirmed enhanced drug localization into the brain tissues following intravenous, nasal and topical treatment.

IT 03

## Multiple Applications of Injectable Hydrogels

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Injectable hydrogels has potential biomedical applications in tissue engineering and regenerative medicine. In our laboratory, we developed injectable shear thinning, bioadhesive, in-situ and self-healing hydrogels for bone regeneration, haemostasis, wound healing and to prevent infections. In this presentation the above-mentioned hydrogel preparation and characterization will be presented. In addition, preclinical studies and relevant applications of the prepared different type of hydrogels will also be discussed in this presentation.

**IT 04**

## Topological and functional analysis of a comprehensive TNFα signalling network

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Tumour necrosis factor α (TNFα) is a pleiotropic cytokine involved in key cellular phenotypic decisions such as death, proliferation, inflammation. Aberrant TNFα signalling is implicated in numerous pathological conditions including autoimmune diseases, neurological disorders, cancer. Appropriate therapeutic strategies to modulate the pathological conditions require insights into the mechanisms governing context-specific phenotypic response to TNFα. Signal transduction culminating in such responses is orchestrated by underlying molecular network of nodes (such as proteins, genes) interconnected by edges (such as protein-protein, protein-gene interactions). Deciphering mechanism(s) controlling specific response requires a holistic approach involving systematic analyses of the TNFα signaling network. In this talk, a novel graph theory and ontology based approach for this purpose will be demonstrated. A comprehensive, well-annotated TNFα network constructed using manual curation, network dimensionality reduction via modularization, and functional annotation of the modules will be presented. Moreover, *in silico* analyses of the (reduced) network to find target interactions, tweaking which may enable modulation of different phenotypes, would be discussed.

**IT 05**

# Biomaterials for Engineering Organotypic Culture Models for Breast Cancer and Cardiac Diseases

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Despite remarkable breakthroughs in biomedical research, further progress in this field is impeded the by lack of in vitro models that mimic the cellular microenvironment in vivo. Animal models are not only expensive but suffer from the limitation of significant differences from human physiology. Moreover, several drugs tested in vitro and in animal models have failed in clinical trials. When cells are cultured in conventional culture platforms such as tissue culture grade polystyrene plates or glass slides their morphology and phenotype is significantly different from what is observed in vivo. The planar 2D architecture and the extraordinarily high stiffness of the substrate fail to mimic the tumour environment. Toward addressing the limitations of conventional 2D culture, we are engineering biomaterials as substrates for tissue culture to probe the underlying molecular mechanisms and for drug screening.

Breast cancer is one of the most common forms of cancer in women and metastasis is the most lethal and clinically challenging stage of breast cancer. We have prepared 3D scaffolds using biodegradable polymers that mimic the stiffness and the architecture of the tumour tissue. MD-MBA-231 cells in the 3D scaffolds exhibit enhanced cell-cell and cell-matrix interactions by 7 days that lead to tumoroids by 14 days than cells in 2D. The cells in the scaffolds also exhibit enhanced markers of stemness and EMT and when injected in mice form invasive and metastatic tumours than the cells from the flat 2D culture plates. Profiling of the global mRNA and miRNA expression revealed that cells in scaffolds better mimic human tumours than cells from 2D.

Cardiac diseases are another major cause of mortality and morbidity worldwide. We have engineered a platform with microscale ridges on silicon to culture neonatal cardiomyocytes to induce alignment, organization and calcium transients, in a manner similar to the native heart. The cardiomyocytes on the engineered substrates were also more responsive to hypertrophic stimuli.

Taken together, the engineered substrates are shown to be better models for culture of breast cancer cells and cadiomyocytes toward developing organotypic models for breast cancer metastasis and cardiac diseases.

**IT 06**

# Blood-based untargeted metabolomics in Relapsing-Remitting Multiple Sclerosis revealed testable therapeutic target

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Relapsing-remitting (RRMS), a most common form of MS, is characterized by acute attacks alternated by partial or complete recovery periods. The major focus of our research is to identify the therapeutic target using metabolomics. Metabolomics is a fast emerging field which can provide a direct "functional readout of the physiological state" of an organism. Identification of blood-based metabolic pathway(s) in relapsing-remitting form of MS (RRMS) which could be used for therapy. Using untargeted ultra-performance liquid and gas mass spectrometry, we measured serum metabolites from 33 RRMS patients, and 14 healthy subjects (HS). A total of 621 known metabolites were detected and 60 metabolites were significantly altered in the serum of RRMS compared to HS. Bioinformatics analysis revealed four metabolic pathways altered in RRMS including glycerophospholipid, citrate cycle, sphingolipids, and pyruvate metabolism. PBMCs isolated from RRMS patients exhibited higher glycolysis suggesting altered metabolic state of immune cells. EAE mice treated with glycolytic inhibitor 2-deoxyglucose (2-DG; once daily), resulted in a significantly delayed ($P<0.001$) the disease progression. 2DG inhibited ($P<0.01$) interleukin 17 production by reducing glycolysis ($P<0.01$) in monocytes of treated EAE group. Using untargeted metabolomic and Seahorse bioanalyzer approaches, we document that RRMS patients showed altered metabolic state "metabotype". Targeting glycolysis, upstream of metabolic pathways altered in RRMS, using pharmacological inhibitor ameliorated the disease progression and pathology in a preclinical model of MS.

**IT 07**

## Porous synthetic matrices as platforms for immunotherapy and cancer studies

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We have developed porous hydrogel matrices and have demonstrated their application as gene delivery or drug screening platforms for immunotherapy or cancer studies. Hydrogels, which are hydrophilic polymer networks, can mimic the physical and mechanical properties of complex three-dimensional (3D) microenvironment of cells and tissues in vivo. We have developed such polymerizable porous hydrogel blends made of polyethylene glycol diacrylate (PEGDA) and gelatin methacrylate (GelMA) and have obtained matrices with tunable properties for varying applications. Characteristics of polymer network greatly influence the morphology and behavior of cells and have been explored to develop a relevant in vitro system for understanding cancer progression and conduct drug studies. Depending upon the blend of the matrix, we have observed spheroidal type of growth or well-spread migratory phenotype of breast cancer cells. Upon culture of cells on these matrices over long periods of time, we have found partial induction of epithelial to mesenchymal transition (EMT) genes in breast cancer cells. We have also tweaked these matrices to improve cell recruitment for gene delivery and immunotherapeutic applications. As part of that, this system is being tested for "in vivo cellular engineering" to recruit T cells and transduce them with T cell receptor via lentiviral gene delivery at the site of implantation. This material-based T-cell therapy could address some of the challenges related to survival and persistence of engineered T-cells encountered with their bolus infusion in context of adoptive T-cell therapy.

**IT 08**

# Avenues of *in vivo* multimodality imaging during development of cancer nanotherapeutics

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Modern biology heavily relies on simultaneous qualitative and quantitative assessments of molecular events in living model systems. Analytical interpretations' using quantitative molecular imaging (MI) is a relatively new field supported by a variety of miniaturized medical imaging tools suitable for application in live cells and/or small animal model systems. By applying photon count based imaging principle, the *in vivo* optical imaging system adds a special flavour in terms of conducting both single cell as well as small animal tissue scale experiments. In oncology research, the role played by miniaturized medical imaging for testing *in vivo* therapeutic efficacies of concept medicines is enormous. Thus the concept of developing theranostic material is on rise, where one molecule serves the dual purpose of therapy and imaging. Gold nanoparticle is one such entity that supports the theranostic concept and thus has gained significant popularity in the field of nanomedicine and nano-diagnostics. My talk will primarily discuss the potentials of gold nanosphere (Au-NS) materials based cancer nanomedicine application. We have shown that novel, biocompatible and photo-disintegrable Au-NS materials, such as Lipos-Au, Au-PLGA [Gold coated Poly-(lactic-co-glycolic acid)], or Au-PNVCL developed for deliberating photo-thermal therapy (PTT) provides highly efficacious therapeutics for cancer cure. Our findings suggest that intra-tumoral delivery of Lipos-Au or even intravenous delivery Au-PLGA nanosphere tuned at 750nm peak absorption can precisely and rapidly ablate tumor mass in preclinical animal model. Focal excitation of low power (650 mW for 4 minutes) near infrared (NIR) laser provides further control in keeping the normal cells at the surrounding margins safe. By attaching NIR fluorescence dye (IR780) on Au-NS material, we have adopted a theranostic approach to study the tumor homing kinetics of the materials. Overall, utilizing multimodality optical imaging toolbox we harness the power of Au-Nanosphere based PTT as a nanomedicine approach.

**IT 10**

## Electrochemical Biosensors for Metabolite Detection

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Electrochemical biosensors have gained increasing importance in the recent years due to the advantages they offer as an analytical tool such as potential for miniaturization, portability, low cost and simplicity of use as compared to conventional solution based assays. Conducting polymer, especially polyaniline [1], has been widely explored for development of electrochemical biosensor due to its ability to act as a good immobilisation matrix for biomolecules such as enzymes, antibodies etc. It also acts as a good transducer and is known to catalyse several redox reactions. Sensing capability of polyaniline based sensors can be enhanced further by preparing its composites with other functional materials such as Prussian blue (PB), metal nanoparticles, CNTs, etc. For *eg.* PB is known to exhibit high catalytic activity and selectivity for reduction of $H_2O_2$, hence PANI-PB composite was used to develop a uric acid sensor which essentially relies on estimation of $H_2O_2$ generated by enzyme catalysed oxidation of uric acid [2]. Polyaniline in nanostructured morphology can provide high interfacial area for efficient immobilization of enzyme and analyte interaction, resulting in improved sensitivity of the biosensor. With this objective, we have synthesized polyaniline nanoparticles and demonstrated its application in glucose sensing [3] and as a supercapacitor electrode material for physiological fluids [4].

More recently, we have developed a novel electrochemical sensor to probe metabolites generated in the microenvironment of live cells in real time [5]. Since cancer cells are known to have abnormal metabolism leading to excessive glycolysis, this sensor can be utilized to differentiate between cancerous and normal cells exploiting the difference in their glycolysis rate. This talk will mainly focus on application of this sensor for cancer detection and for evaluating efficacy of glycolysis inhibiting anti-cancer drugs. Furthermore, results of our research on detection of cancer biomarkers using surface plasmon resonance technique will be discussed. To summarize, this talk will present an overview of our efforts in designing electrochemical biosensor for detection of metabolites from the point of view of medical diagnostics.

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**IT 11**

# miRNA regulation of stem cell differentiation: Do miRNA networks regulate signalling networks in differentiating Mesenchymal Stromal Cells?

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A number of studies have shown that individual miRNAs regulate MSC differentiation especially into the chondrogenic lineage. Our group has earlier shown that miRNA networks regulate gene networks in human embryonic stem cells derived MSC expanded in culture (Koh BMC Genomics 2010). However it is unclear if miRNAs at physiological levels regulate MSC differentiation by regulating specific signalling pathways involved in MSC differentiation. We have earlier shown that TGF-b signaling is critical for MSC growth and differentiation (Ng Blood 2008). To understand the role of miRNAs in regulating TGF-b signalling, we compared miRNA expression of foetal limb MSC treated with SB431542, a compound that inhibits TGF-b signalling through the Activin-Nodal arm of the pathway. We observed distinct sets of miRNAs whose expression changed in response to inhibition of TGF-b signaling in MSCs differentiating into osteogenic and chondrogenic lineages, but not adipogenic lineage. We further correlated these changes in miRNA expression with changes in expression of their predicted mRNA targets from the same sample to identify signalling networks regulated by these miRNAs.

**IT 12**

# Identification and Analysis of KIX domains and their Interacting partner Transactivation Domains (TAD) during Transcription

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Transcription factors are central regulatory proteins in organismal development, with the ability to activate or repress gene expression by recognizing highly specific cis-regulatory elements on DNA. Two of the main functional sites in TFs are the DNA Binding Domain (DBD) and the Transactivation Domain (TAD). DBDs provide recognition sites on transcription factors through which they bind to enhancer or promoter regions on DNA while TADs are small sticky regions that bind to co-regulators or co-activators, which further associate with RNA polymerase and initiate the transcription process. One such co-activator is the KIX domain, first identified in CREB-Binding Protein (CBP) of mouse, now established to be a major regulatory domain of the transcription process in yeast and mammals. Structurally, it is a small triple helix domain that has been shown as the recognition and binding site of TADs in a range of transcription factors. TADs are often intrinsically disordered, gaining stable secondary structure only after binding to KIX. Although some of the KIX-TAD interactions are well characterized in mammals and yeast, the molecular basis of KIX-TAD interactions in plants is yet to be explored. Huge gaps exist in the structural knowledge of KIX as well as TAD domains, with practically no reports of the biophysical KIX-TAD interactions, particularly for plants. The focus of this work is the identification, characterization and analysis of KIX domains and their interaction partners, the TADs, via computational approaches like hidden markov models and machine learning classifers, followed by investigation of their binding interface via structural modelling, and finally, experimental validation of our predictions.

**IT 13**

## Realization of Hydrogen Economy with Electrochemical Energy Devices

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Hydrogen economy is the sustainable production and utilization of hydrogen and shifting to hydrogen economy has the potential to reduce the carbon footprint substantially. The production of hydrogen, the first part of hydrogen economy is typically achieved by electrochemical and photoelectrochemical water splitting reactions. These reactions are energy demanding catalytic reactions and enormous efforts are dedicated across the globe to invent new catalysts and combinations to reduce the overpotential to economically accessible levels. The fact remains that hydrogen production is still an expensive electrochemical reaction and we aim to realize the hydrogen economy in energy devices such as fuel cell and batteries by tailoring electrochemical interfaces. Hydrogen generation can be induced in fuel cells by harvesting the heat of neutralization and in batteries by catalytic mediation. Hydrogen generation as well utilization or hydrogen economy can be realized by utilizing the proton coupled electron transfer in hydrogen storage molecules.

**IT 14**

## Systems driven Synthetic bio therapeutics device in Leishmaniasis

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The work revolves around modulating signaling in *Leishmania* infected macrophages. Till date, leishmaniasis is treated with traditional pharmaceutical approaches. Newer approaches to modify the host action against the parasite would be a better option to resolve the *Leishmanial* parasite. The strategies adopted helped devise an immuno-modulatory synthetic signaling circuit targeting CD14-TNF and EGFR pathways in Leishmaniasis. When macrophages are infected with *Leishmania,* multiple signaling inputs arrive simultaneously and/or sequentially, that are subsequently integrated for an anti-inflammatory pathophysiology in leishmaniasis. Novel biological devices may be constructed, that revert these signals for a pro-inflammatory leishmanicidal response to curb infection. CD14, TNF and EGFR pathways has been considered for dynamical system theory analysis, whose parameters were fitted within the known biological limits for a desired and predictable system behavior (BIOMD0000000477). Network metrices indicate that the signaling cascade is a real world network with crosstalk points MKK1/2, MKK3/6, MKK4/7 and IKK–NFkB, central to modulations for different phenotypic responses. Furthermore, the downstream gene network of CD14-TNF-EGFR pathway was reconstructed. Network analysis showed that NFkB links the signaling and gene network, used as a point of intervention through a synthetic circuit embedded within the negative autoregulatory feedback loop. A chimeric protein kinase C (PKC) was incorporated in the synthetic circuit, under the transcriptional regulation of Lac repressor and IPTG, as an inducer. The chimeric PKC via IKKb phosphorylation activates NFkB, and modulates the gene expression from an anti-inflammatory to a pro-inflammatory phenotype in *in vitro L. major* infected macrophage model.

**IT 15**

## Disease-responsive biomaterials: A novel concept for the treatment of autoimmune and inflammatory diseases

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A significant leap in drug delivery is an autonomous system that titrates the amount of drug released in response to a disease, for instance, inflammation, ensuring the drug is released only when needed at therapeutically relevant concentration. Diseases have inherently fluctuated in nature such as inflammatory and autoimmune diseases, in particular, pose an enormous challenge to deliver drugs in safe, efficient and compliant manner. In what follows we will take a brief look at current approaches about biomaterials-based therapeutics and with examples taken from our work to examine how disease-responsive biomaterials have developed to i) improve the lifetime of the transplanted organs, ii) locally injectable hydrogels for the treatment of inflammatory arthritis, and iii) inflammation-targeted drug delivery to alleviate inflammatory bowel diseases.

IT 16

## Affordable Healthcare Technologies

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There is an increasing demand for accurate, efficient and cost-effective treatment methods and devices in healthcare. The main goal behind the research in Nanobios Lab at IIT Bombay relates to the development of biosensor assays and their integration into affordable Point-of-care diagnostic devices and use of nanoengineering techniques for affordable healthcare products.

Nanobios lab in collaboration with Biosense Technologies Pvt Ltd have already commercialized, uChek (http://uchek.in) - a low cost smartphone based urine dipstick reader which was designed, tested and deployed. uChek can interpret upto ten analytes in urine including glucose, bilirubin , ketones, proteins, urobilinogen, pH, SG, occult blood, leukocytes and nitrites. The accuracy of uChek was found to be comparable to commercially available semi-automated urinalysis instruments in laboratories with 100% of readings within +/- 1 color block.

Nanobios lab in collaboration with Biosense Technologies Pvt Ltd have also manufactured and commercialized "SuChek". Suchek is an indigenous, accurate, low-cost glucometer supported by the Indian Council of Medical Research. Suchek reagent strips are as accurate as conventional glucometers, at a fraction of the price. Along with the glucometer, the companion Suchek mobile application helps save, trend and analyze blood glucose levels at an individual level or track response to treatment at a community level.

Microneedles are being fabricated in the lab for delivery of vaccines and drugs. We believe effective care of the most hard-to-treat conditions requires approaches beyond simply taking medicine / applying patch. We are transforming how medicine is delivered and how people achieve their health goals through the convergence of optimized drug delivery, embedded sensor technology to monitor compliance, and connected and personalized behavioral support.

Another project involves the design of a heat triggered Transdermal drug delivery system (TDDS) using a thermoresponsive gel patch, where patients can themselves administer a pulse of drug on mere application of heat pad over the TDDS, whenever pain is experienced. We have also created novel drug loaded sponges for combating Surgical Site Infections (SSI). SSIs are best prevented by eradicating bacteria at the earliest stage, by deploying effective counter-measures locally so that bacteria does not propagate further and cause infection at the operated site. Finally, we have also developed bioresorbable bone screws of novel biomaterial composite materials with advanced functionality and improved design that are now moving to large animal trials.

We believe that these are small steps towards “Make in India and Made in India” and a lot more needs to be done to educate everyone of the importance of making affordable healthcare products in India.

# ORAL TALKS

**OT 01**

# Peripheral nerve fibres within thick-skin as a route for nanoparticle delivery

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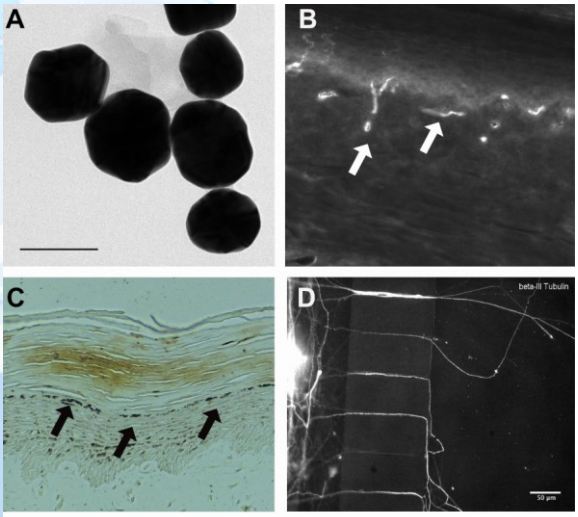
Nerve fibers innervating the skin are terminal axons originating from neuronal cell bodies located at distal ganglia. These fibers form 'pathways' that can be utilized to access neurons to treat diseases such as small fiber neuropathies, chronic pain conditions, and nerve injury. The thick-skin covering the palms and soles is densely innervated by sensory nerve fibers, making them a potential therapeutic target. However, these fibers are embedded in deeper layers of the epidermis and dermis, making them difficult to access(1). Nanoparticle-based drug delivery across skin and to epidermal nerve fibers have much translational applications, but nanoparticle penetration especially through thick-skin, is not clear. This study specifically investigates the effectiveness of gold nanoparticles (AuNPs) for thick- skin penetration, especially across the stratum corneum (SC) as a function of particle size and determines the uptake of such particles from peripheral axons. Epidermal penetration of AuNPs was characterized both, in harvested skin from the hind-paw using a diffusion chamber, as well as in vivo. Peripheral axons cultured in microfluidic devices were utilized to determine nanoparticle uptake into sensory neurons. In animal studies, hind-paw skin of adult rats exposed to AuNPs solution for 3h, demonstrated nanoparticles in blood on the 4th day, and histological analysis revealed AuNPs in epidermal layers just below the SC, with no apparent tissue response(2). We conclude that the thick-skin allows nanoparticle penetration and acts as a depot for release of AuNPs into circulation long after the initial exposure has ceased. We also observe that transdermally applied nanoparticles has the potential to be used for targeting epidermal nerve fibers.




Representative images of synthesized gold nanoparticles of 100 nm size (A), skin sections demonstrating intra-epidermal nerve fibres (B), gold nanoparticle penetration in rat hid-paw skin (C), and microfluidic system with axo-somal separation (D).

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**OT 02**

## Large-scale analysis of protein thermostability and detergent tolerance

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Understanding how structure and activity of proteins are related to the proteins' (thermo-)stability or tolerance against solvents and detergents is of utmost importance in protein engineering. However, until now, the role and impact of the location and type of substitution on protein properties has been predominantly revealed from analyses of only a few protein variants or large-scale studies over data sets of many proteins. Furthermore, the majority of analyses considered only one protein property at a time. Here, for the first time, we exhaustively characterize changes in thermostability *and* detergent tolerance for a complete site-saturation mutagenesis library containing 3439 single variants of the *Bacillus subtilis* lipase A. To establish a set of generally applicable guidelines regarding improved protein thermostability *and* / *or* detergent tolerance, we combined hot spot identification, investigation of protein structural characteristics, and screening of the variants via rigidity theory-based CNA (Constraint Network Analysis; Figure 1) (1). The main outcome is that CNA can successfully predict hot spots prospectively in a rational proteisn design approach aiming at improved protein thermostability *and* detergent tolerance.

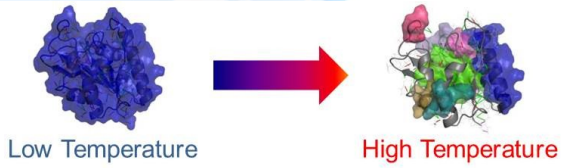


Figure 1: Rigidity theory-based analysis of *Bs*LipA.

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**OT 03**

# Smart magnetic sensors and Development of a magnetoresistive biosensor for the detection of biomolecules

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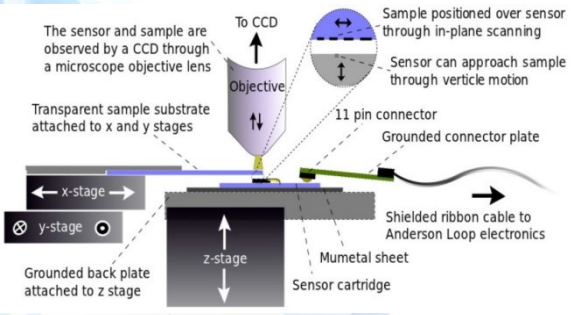
Magnetic sensors play an essential role in modern technology. They are widely used in nearly all engineering and industrial sectors, such as high-density magnetic recording, navigation, military and security, target detection and tracking, antitheft systems, nondestructive testing, magnetic marking and labeling, geomagnetic measurements, space research, measurements of magnetic fields onboard spacecraft and biomagnetic measurements in the human body.

A versatile stand-alone TMR-scanning microscope as magnetic scanning instrument is developed, with mapping capabilities. The platform as a whole is suitable for studying magnetic carriers of various types, such as for magnetosome imaging in magnetotactic bacteria or other micron-sized magnetic entities.

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**OT 04**

# Small angle scattering studies of solid lipid nanoparticles in solution

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We have recently reported a novel microwave-assisted microemulsion technique for the production of solid lipid nanoparticles (SLNs) (1). Suspensions of SLNs stabilized with emulsifiers have been extensively investigated as drug carriers since the 1990s, although details of their ultrastructure are poorly defined.

We further employed multi-angle static and dynamic light scattering (SLS/DLS), small angle X-ray and neutron scattering (SAXS/SANS) techniques to help elucidate the micro- and ultrastructure of microwave-produced SLNs. The SANS technique was used to probe the hierarchical structure of SLNs (2).

The SLS/DLS data indicate a core–shell structure with a shell thickness of ~130 Å. SAXS data suggest that the SLNs have a lipid lamellar structure with a repeat spacing of 41.0 ± 0.1 Å (3).

The SANS results indicate SLNs with a multi-length scale structure and polydisperse large particles with roughened surfaces at the microscale level. At the nanoscale level, the SLNs have an ellipsoidal shape intermediate between spheres and rods, with a crossover from mass fractals to surface fractals (3).

The elucidation of SLN structure is particularly important given that the structure influences the stability and drug release properties of the nanoparticles. These results and further exploration will further our understanding of the SLN structure and aid in engineering of particles to impart controlled release properties to SLNs.

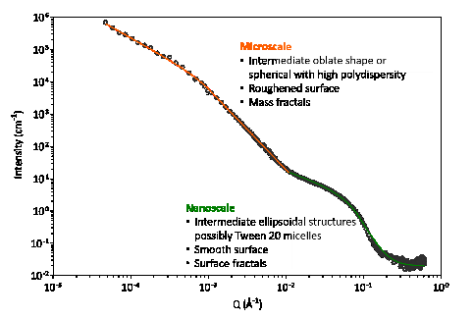


Figure (1): USANS/SANS data from SLNs.

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***Keywords**: solid lipid nanoparticles, small angle X-ray scattering, small angle neutron scattering, light scattering, drug release, ellipsoidal model.*

**OT 05**

## Graphene-structured materials for highly active and durable oxygen reduction electrocatalyst

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Increasing demand for highly enhanced energy conversion and storage devices continually mount as humans continue to increase energy consumption, rendering next generation energy materials a crucial technology for a clean and sustainable future. The electrocatalytic oxygen reduction reaction (ORR) is one of the most important reactions for electrochemical conversion and energy storage technologies, such as fuel cells and metal-air batteries. In this talk, I will discuss the direct synthesis of graphene-structured materials for ORR. I will share some of my recent results on large-area mesoporous-structured Pt thin film on ionic polymer-doped graphene (MPt/IPG) as a highly stable electrocatalyst for the ORR. With the great advantages of strong interfacial cohesion arising from ionic block copolymer as an interfacial linker, I will also discuss about the development of Mo-PdPt@Pt octahedra decorated with ionic block copolymer-functionalized rGO. We believe that our robust concept of newly developed MPt/IPG, Mo-PdPt@Pt core-shell octahedra may overcome the activity and durability issues reported for previous Pt-based electrocatalysts.

OT 06

# DNA Based Emerging Technologies for Biological Applications

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Structural DNA nanotechnology explores various nanoscale structural and functional properties of DNA to manipulate matter at nanoscale for diverse applications1. Three-dimensional architectures based on DNA polyhedra have raised particular interest in biomedical applications2. DNA polyhedra possess an internal void bounded by a well-defined three-dimensionally structured surface3. The internal void can house cargo, and the designer DNA scaffold can facilitate molecular display to program biological targeting. While the delivery of designer DNA particles bearing surface ligands has been achieved4, the successful demonstration of their full potential of targeted delivery when housing an internal payload remains an outstanding challenge. I will present the first successful delivery of quantum dots (QDs) as the internal payload of DNA icosahedra. A long- standing challenge for QDs has been the inability to achieve their monofunctionalization in bulk5. We resolve this by encapsulating QDs within molecularly identical icosahedral DNA particles in bulk where the DNA shell is mono-functionalized with different endocytic ligands. We demonstrate the monofunctionalization and successful specific, endocytic uptake of QDs, using multiple endocytic ligands like folic acid, Galectin-3 (Gal36) and Shiga toxin B-subunit (STxB7). Single particle tracking of Gal3/STxB-bearing, QD-loaded icosahedra reveal new observations of compartment dynamics along the endocytic pathways. QD-loaded DNA polyhedra bearing ligands of unique stoichiometry represent a new class of high-precision molecular imaging tools for quantitative approaches to complex biological phenomena arising from receptor clustering8-10. Our results highlight the emerging potential of DNA devices in cell biology and biomedical applications that could enable probing and programming various biological systems as well as developing next generation tools for targeted delivery of molecular payloads within living systems.

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***Keywords**: DNA Nanotechnology, Quantum dots, Monofunctionalization, Bioimaging, Targeted Delivery.*

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**OT 07**

# Development of electrochemical nano-immunosensor for early detection of hepatocellular carcinoma

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Hepatocellular carcinoma (HCC) is one of the most common lethal cancers worldwide. Hepatitis inflammation and cirrhosis remains the major etiologic agents of liver neoplasm [1]. Existing screening methodologies include protein biomarker detection by enzyme-linked immunosorbent assay or radioimmunoassay and imaging techniques. However, imaging modalities cannot differentiate between cancerous masses [2]. Till now, alpha-fetoprotein (AFP) remains clinically validated biomarker for HCC diagnosis. But, it cannot be considered as a perfect diagnostic test since its elevations are also associated with germ cell and gastrointestinal tumours [1]. Therefore, in this study, we selected a potent HCC-specific biomarker glypican-3 (GPC-3) in combination with AFP. GPC-3 is a promising research biomarker in distinguishing benign, normal and cancerous HCC lesions [1]. In this work, a point-of-care diagnostic platform is constructed based on dendrimer functionalized magnetic nanoparticles (Fe3O4 NPs). Dendrimers are three-dimensional nanostructures that not only provide stability to Fe3O4 NPs but also help in binding biological ligands to the surface of colloids. The superparamagnetic behaviour of Fe3O4 NPs enhances magnetoseparation process to increase sensitivity of the biosensing process. The Fe3O4 NPs are surface functionalized with amine-terminated polyamido-amine (PAMAM) dendrimers by chemical co-precipitation method. The synthesized nanoparticles are characterized using FT-IR, XRD, VSM and TEM. Antibodies (anti-AFP and anti-GPC-3) are immobilized onto the dendrimer-magnetic nanosurface using gluteraldehyde as a cross-linking agent.The proposed immunosensor is electrochemically characterized using cyclic voltammetry, differential pulse voltammetry (DPV) and electrochemical impedance spectroscopy. Redox mediators; prussian blue and toluidine blue was utilized for simultaneous detection of AFP and GPC-3, respectively by DPV. Under optimal conditions, immunosensor exhibited a wide linear range of 0.02 to 100 ng/mL with a low detection limit of 0.05 and 0.07 ng/mL for AFP and GPC-3 respectively. The present strategy holds enormous clinical significance towards more sensitive, specific and early HCC diagnosis.

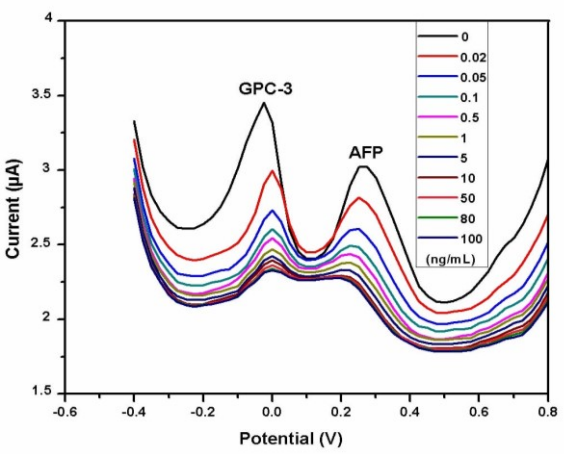


Figure (1): DPV's of AFP and GPC-3 immunosensor after incubation with different concentration of respective antigen

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***Keywords**: HCC, dendrimer, magnetic nanoparticles,, electrochemical immunosensor, AFP, GPC-3*

**OT 08**

# Therapeutic evaluation of magnetic liposomes engineered for self-controlled hyperthermia and chemotherapy

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Magnetic liposome-mediated combined chemotherapy and hyperthermia is gaining importance as an effective therapeutic modality for cancer. But, controlling and maintenance of hyperthermia temperature is a major challenge in clinical settings due to the overheating of tissues. To overcome this problem, we developed a novel magnetic liposomes formulation co-entrapping a dextran coated biphasic suspension of $La_{0.75}Sr_{0.25}MnO_3$ (LSMO) and iron oxide ($Fe_3O_4$) nanoparticles for self-controlled hyperthermia and chemotherapy. In this work, *in vivo* biocompatibility and therapeutic evaluation studies of the novel magnetic liposomes are reported. Biocompatibility study of the magnetic liposomes formulation was carried out to evaluate the signs of preliminary systemic toxicity, if any, following intravenous administration of the magnetic liposomes in Swiss mice. Therapeutic efficacy of the magnetic liposomes formulation was evaluated in the fibrosarcoma tumour bearing mouse model. Fibrosarcoma tumour-bearing mice were subjected to hyperthermia following intratumoral injection of single or double doses of the magnetic liposomes with or without chemotherapeutic drug paclitaxel. Hyperthermia (three spurts, each at 3 days interval) with drug loaded magnetic liposomes following single dose administration reduced the growth of tumours by 2.5 fold whereas the double dose treatment reduced the tumour growth by 3.6 fold compared to their corresponding control. At the end of the tumour efficacy studies, presence of MNPs was studied in the remnant tumour tissues and vital organs of the mice. No significant leaching or drainage of the MNPs from the tumour to the other vital organs of the body was observed, suggesting again the potential of the novel magnetic liposomes formulation for possibility of developing as an effective modality for treatment of drug resistant or physiologically vulnerable cancer.

***Keywords:*** *Magnetic nanoparticles, cancer hyperthermia, liposomes, biphasic suspension*

**OT 09**

# Preparation and evaluation of bioactive glass scaffolds containing levonorgestrel by 3D printing approach for bone tissue regeneration.

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Large bone defects occur because of multiple myeloma, osteoporosis, traumas, brittle bone diseases, high energy injuries, certain types of cancers like osteosarcoma. First visible sign amongst all these is bone fractures. In present study LNG loaded mesoporous bioactive glass (MBG) was synthesised & characterised. LNG is believed to act by accelerating osteoblast formation. 3D printing technique was used to prepare a scaffold. The scaffolds were evaluated for porosity. *In-vitro* biomineralisation studies were carried out for 1 month to study the formation of hydroxyapatite (HA) which was able to produce hydroxyapatite (HA) at the interface of natural bone and bioactive glass surface when implanted.Drug release studies from the scaffolds were carried out which indicated that slow release of drug takes place at various intervals of time. Drug release was not hindered by simultaneous formation of hydroxyl-carbonated apatite (HCA). The *in–vivo* studies were performed by implanting sterilised 3D printed scaffolds, in feromal defect model in rats. The studies were performed as per approved IAEC certified protocol. The bones of rats were evaluated for osteoblast formation by histopathological studies. The results indicated that BMG scaffolds loaded with LNG fabricated by 3D printing has significant increased osteoprogenitor activity compared to BMG scaffolds without LNG. This combination of 3D printed scaffold along with LNG loaded on it will have synergistic action in treatment of postmenopusal osteoporosis as it will prevent further bone loss as well as regeneration of load bearing bones by stimulating osteoblast activity and osteocalcin formation.

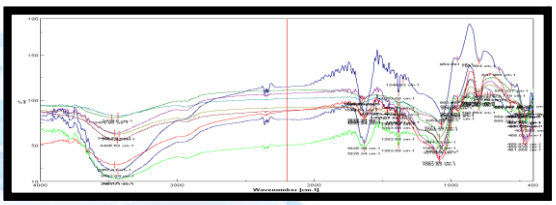

Fig. 1: Cumulative drug release curve.

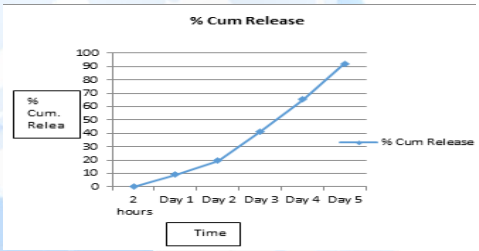


Fig. 2: FTIR overlay of *in-vitro* bio mineralization studies in SBF.

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***Keywords:*** *Mesoporous bioactive glass, 3D printing, HA, HCA, Levonorgestrel, In-vitro biomineralisation, Osteoblast.*

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**OT 10**

# Folic acid conjugated arsenic trioxide nanoparticles for improved drug delivery

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Medicinal use of arsenic and its derivatives dates back to more than 2400 years. Arsenic and its derivatives have been known for their antiseptic, depilatory, antispasmodic and tonic properties since ancient times1. These occur in numerous forms and exhibit wide applications ranging from remedial to therapeutic. The approval of arsenic trioxide (As2O3) by the United States Food and Drug Administration (USFDA) for the treatment of acute promyelocytic leukemia in newly diagnosed and relapsed patients brought As2O3 the status of a medicine. The remarkable efficiency of As2O3 in haematological cancers encouraged researchers to study its effect on other solid tumors. However, the drug was found to cause severe toxicity, gastrointestinal upset, hyperglycaemia, rash, itching and tachycardia. This necessitated developing strategies for improved formulations of this potent drug with reduced adverse effects.

Folate receptors (FR) are highly over-expressed in many tumor types2. This fact can be exploited to target imaging molecules and therapeutic drugs directly to cancerous tissues with minimal or no harm to normal cells. Folic acid (FA) as one of the most popular ligands retains a high affinity for its receptor. Therefore, FA and folate conjugates have demonstrated significantly enhanced delivery to FR-positive tumor cells.

In the present work, we developed As2O3 NP conjugated with FA for improving the therapeutic drug delivery. Ex-situ synthesis method was adopted which is a simple, cost-effective and robust method. Further characterization by Fourier transformed infrared spectroscopy (FT-IR), X-ray diffraction (XRD), Ultraviolet-visible (UV-vis) spectra, inductively coupled plasma-atomic emission spectrometer (ICP-AES), zeta potential and transmission electron microscopy (TEM) was done.

Safety of the FA-As2O3 nanoparticles was assessed using haemolysis and blood cell aggregation studies. FA-As2O3NPs were assessed for their biocompatibility using non-cancerous cell lines by time- and dose-dependent cytocompatibility MTT assay. Molecular simulation studies provided evidence of interaction between FA and As2O3. Our work demonstrates that the obtained FA-As2O3 nanoparticles could be effectively used for potential delivery of As2O3 to cancer cells.

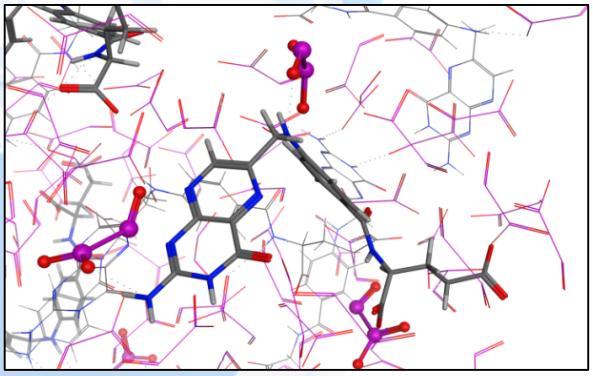

Figure (1): Binding mode of As2O3 and folic acid (PDB ID 4Z7F). 3D picture depicting the binding mode of As2O3 (red and purple ball-and-stick model) with folic acid (blue and grey white ball-and-stick model)

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***Keywords**: Arsenic trioxide nanoparticles, Folic acid, Haemolysis, Blood cell aggregation, Cytotoxicity, Biocompatibility, Molecular simulation studies.*

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**OT 11**

# Self-assembled levodopa tubes mediated synthesis of Au microroses as SERS probes in C6 glioma cells

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**Background:** Motivated by multifaceted, intricate methods reported in literature, herein, we report a novel notion of assembly dependent single step synthesis scheme for the high yield fabrication of stable gold microroses, which simply involves manual mixing of chloroauric acid and self-build levodopa microtubes at room temperature.
**Method:** The study reports a novel and simple synthesis procedure for the fabrication of self-assembled levodopa microtubes and Au microroses along with influence of various process parameters. We also demonstrate the potential application of Au microroses towards SERS based detection of biomolecules in cells.
**Results:** Firstly, the tube forming ability of levodopa is being explored, next, the role of levodopa tubes in the fabrication of Au microroses.

Dynamic light scattering analysis revealed that Au microroses had an average hydrodynamic size of 1.23 ± 0.14 µm with a tight polydispersity index of 0.298 ± 0.06 and zeta potential of -28.5 mV. Scanning electron microscopy micrographs showed that Au microroses were extremely monodispersed having mean diameter of 1.28 ± 0.28 µm with numerous undulations on their surface, i.e. petal like structures with observed thickness of 62.8 nm and approximate length of 963.2 nm. Transmission electron microscopy micrographs showed a coating over the petals of about 2.5 nm, which could be attributed to the levodopa and its oxidized products i.e. 5, 6-dihydroxyindole.

A magnified high resolution transmission electron microscopy image indicated that the petals were highly crystalline. The lattice spacing was 0.236 nm, which matched with Au (111) planes d-spacing, indicating both single crystallinity and multiple (111) facets.
Au microroses show an intense SERS spectrum upon capping with rhodamine (R6G) molecules even at a low concentration. The increased intensities of bands at 1363 $cm^{-1}$ and 1573 $cm^{-1}$ were observed. C6 glioma cells were incubated with R6G, Au microroses and R6G capped Au microroses to investigate the SERS effects. Typical SERS bands of 1355 and 1570 $cm^{-1}$, was clearly observed.
**Conclusion:** The system is facile, controllable, reproducible, and 100% aqueous with enhanced stability. The unique structure of microroses accompanied by abundance of nano-textured sheets coated with oxidize products of levodopa offer numerous interaction sites for the biomolecules as well as cells, thereby making the system a favorable bio-sensor. The novel system may find wide applications in catalysis, drug delivery systems etc.

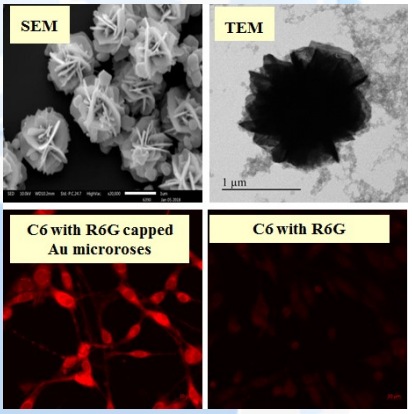


Figure (1): SEM, TEM micrographs of the formed microroses, and their cellular uptake in C6 cells.

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***Keywords**: self-assembly, levodopa tubes, gold nanoroses, one-pot synthesis*

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**OT 12**

# Highly Monodisperse Dendritic Fibrous Nanosilica: Scalable Synthesis Quantified by E-Factor and Applications in Lasing by Self-Assembled Photonic Crystals

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Although the field of nanomaterial synthesis has expanded over last two decades with the innovation of many unique morphology-controlled nanostructures, such as dendritic fibrous nanosilica (DFNS), their successful use hinges critically on the development of scalable synthesis methods to provide technologically significant quantities of high-quality nanomaterials with tunable size, morphology and textural properties. This study details a simple, versatile, scalable synthesis route for DFNS. We develop a DFNS synthesis process by replacing the microwave-assisted close-reactor synthesis protocol with a round bottom flask-based open reactor protocol[1-4]. This development not only enhances the sustainability of the process but also allows the synthesis of highly monodispersed DFNS with a narrow pore size distribution and controllable particle size, fiber density and textural properties. The DFNS were highly mono-disperse and readily formed colored photonic crystals. Moreover, their photonic band gap was tunable by using different types of DFNS (varying in size and fiber density), which can be used to harvest light in various applications. Photonic Crystals of DFNS have shown unique lasing action which is not only depend on their sizes but surprisingly also on their fiber density. The sustainability of this protocol was compared with nanomaterial synthesis protocols for a range of nanomaterials using the E-factor, and we found an exceptional E-factor value of 15 for the DFNS protocol, which is several orders of magnitude better than other reported processes.

Table (1): Comparison of E-factors for various nanoparticles.

| S. No. | Nanomaterial | Synthesis Protocol | E-factor | Ref. |
|---|---|---|---|---|
| 1 | Fibrous nanosilica (DFNS-6) | Hydrolysis-condensation | 15 | This work |
| 2 | Titanium dioxide | Hydrolysis-calcination | 17800 | 5 |
| 3 | Carbon nanotubes | Chemical vapor deposition | 170 | 5 |
| 4 | Fullerenes | Benzene-oxygen flame | 950 | 5 |
| 5 | Gold NPs | Phosphine-stabilized | 7200 | 5 |
| 6 | Gold NPs | Thiol-functionalized ionic liquid | 99400 | 5 |
| 7 | Gold NPs | Starch-glucose | 29600 | 5 |

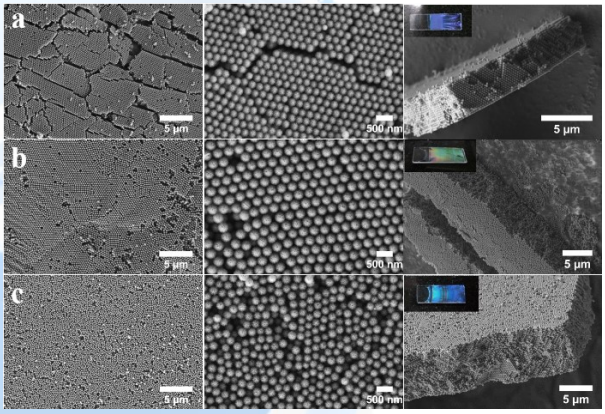


Figure (1): SEM images of photonic crystals of various DFNS, a) DFNS-6 b) DFNS-9 c) DFNS-12. In inset, optical photograph.

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***Keywords***: *Dendritic Fibrous nanosilica, Sustainable Synthesis, E-factor, Photonic Crystal, Lasing.*

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**OT 13**

# Real-Time Metabolic Interactions between Two Bacterial Species Using a Carbon-Based pH and Peroxide Microsensors as a Scanning Electrochemical Microscopy Probes

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Scanning Electrochemical Microscopy (SECM) is used to study the local chemical environment above live bacterial biofilms such as S. gordonii (Sg), S. mutans (Sm) etc. In this study, we report the development of a Pt decorated carbon nanotubes (CNTs) based dual SECM probe to detect low micro-molar range hydrogen peroxide ($H_2O_2$) produced by the live bacterial biofilm. This sensor showed sensitivity 2.2 ± 5 mA $cm^{-2}$ $mM^{-1}$ with low detection limit of 0.5 µM. Our results indicate that the Sg produced 65-70 µM $H_2O_2$ within 30 min in presence of 1 mM glucose in artificial saliva solution (pH 7.2) at 37°C. In addition, we have also developed a unique solid state carbon based potentiometric pH sensor and used as a SECM probe to map the pH change at high spatial resolution above the Sg biofilm. The sensor showed Nernstian response with slope of 58±4 and very fast response time of 5s. The pH mapping above the biofilm showed that pH above the biofilm dropped by one pH unit within 30 min only in 6 pH artificial saliva with 30 mM sucrose at 37°C.

We discovered that the production of $H_2O_2$ by Sg was suppressed by the immediate presence of acid producing bacteria, Sm. The results suggest that $H_2O_2$-producing bacteria such as Sg are dominant while the buffering capacity of the saliva is still valid (~pH 6.0−7.2), but that Sm gradually takes over by decreasing the local pH to 5.0 or less through lactic acid production. The unique capabilities of SECM, combined with a micro-sized ion-selective electrode or pH probe and peroxide probe, in quantitative chemical mapping with high spatial resolution makes it a powerful tool in the investigation of these bacterial metabolic interactions.

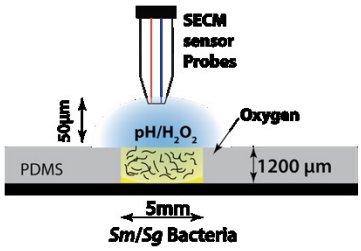


Figure (1): Schematics representation of bacteria biofilm substrate with scanning electrochemical microscopic (SECM) probe.

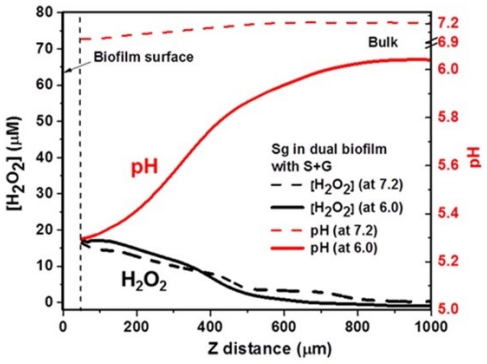


Figure (2): Z-direction $H_2O_2$ and pH profile from 50 µm above Sg in the dual-bacteria biofilm to 1000 µm above in the bulk solution in the presence of carbohydrates at pH 6.0 (solid lines) and 7.2 (dashed lines).

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***Keywords**: Scanning electrochemical microscopy, S. gordonii, S. mutans, electrochemical biosensors.*

**OT 14**

## Interfacial modification of inorganic nanoparticles for drug delivery applications

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Recent advances in nanotechnology play an important role in designing nanocarriers with specific functional properties that can address the shortcomings in the area of anticancer drug delivery. Among the others, $Fe_3O_4$ and CuS nanocarriers possess unique physio-chemical properties with an ability to get functionalized at molecular and cellular level.

In this talk, the design and development of pH responsive $Fe_3O_4$ nanocarriers that are amenable for drug delivery applications will be discussed. It has been observed that interfacial modification of the surface of $Fe_3O_4$ nanocarriers allows us to create functionalized exterior with high densities of organic moieties for conjugation of drug molecules and biolebelling. These nanocarriers have an average size of about 10 nm and possess tunable surface charge properties. The interfacial modfication of nanocarriers were investigated by various sophisticated instruments such as infrared spectroscopy, dynamic light scattering, zeta-potential and thermogravi-metric measurements etc. These nanocarriers were used for loading of both hydrophilic and hydrophobicanticancer agents (doxorubicin hydrochloride methotrexate and curcumin). The drug loaded nanocarriers exhibit good cellular internalization and substantial toxicity to cancer cells. Specifically, the high loading affinity of these nanocarriers for anticancer drugs (doxorubicin hydrochloride, methotrexate, curcumin), their pH dependent sustained release profile, low toxicity and good cellular internalization make these nanocarriers suitable for drug delivery applications. Further, receptor conjugated magnetic nanoparticles and fluorescent magnetic nanohybrids have received a great deal of attention due to their potential applications in intracellular drug targeting and cellular imaging. The development of a new class of aqueous stabilized, biocompatible $Fe_3O_4$ decorated $YPO_4$: Eu nanohybrids and folate conjugated $Fe_3O_4$ bifunctional nanoparticles will also be discussed.

In addition to this, CuS nanocarriers having capability to deliver anticancer durg as well as photothermal therapy will be presented. Specifically, glutathione (GSH) functionalized CuS nanocarriers (absorption near infrared region) showed good heating efficacy under NIR laser were developed. It was found that the temperature of the aqueous solution of GSH-CuS nanocarriers increases from 27.

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**OT 15**

## A Rechargeable Hydrogen Battery

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Hydrogen, the most abundant element in universe is well known as clean energy source for decades[1]. Here we formulate A Rechargeable Hydrogen Battery for the first time. We are demonstrating a reversible energy conversion system, which shuttles $H^+$- ion back and forth during charging and discharging respectively, with the regain of consumed hydrogen during charging. This was successfully attained by exploiting the hydrogenation and dehydrogenation of simple Quinone (Figure 1), which is environmentally benign and economic organic molecules. Electrochemical, spectroscopic and spectroelctrochemical analysis show the participation of protons during charge–discharge and extended cycling[2]. We believe that this concept based on a virtually non-polluting energy carrier molecule adds a compelling piece to the sustainable energy puzzle.

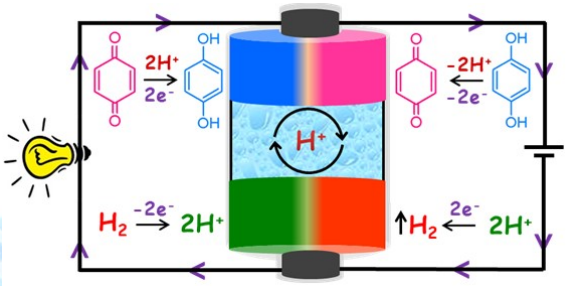


Figure (1): Schematic Representation of a Rechargeable Hydrogen Battery Based on a Hydrogen-Storing Quinone/ Hydroquinone Redox System

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***Keywords***: *Electrochemical Hydrogenation, Hydrogen Storage Molecule, Proton Coupled Electron Transfer, Hydrogen Evolution Reaction, Rechargeable Hydrogen Battery*

# POSTER PRESENTATIONS

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**NDDT 01**

# Tunable scaffold based biomaterial as a model for delivering drugs for bacteremia

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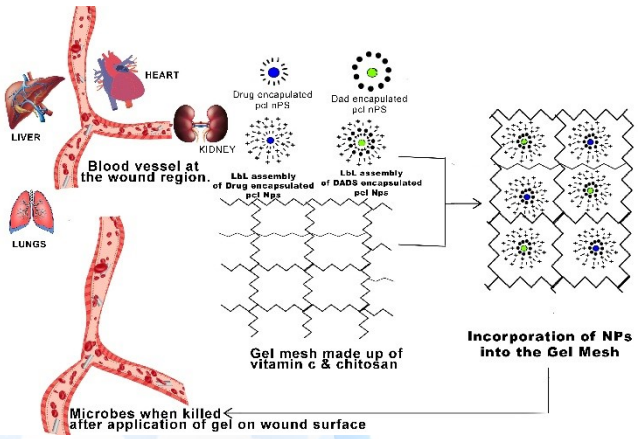
**Background:**
Bacteremia is often a life intimidating serious disorder affecting millions of life in no time. This is often a reported cause for alarming death rates all over the world. The etiology associated with the disorder includes invasion of bacteria into bloodstream where bacteria is resistant towards currently used antibiotics. Currently, hospital associated bacteremia occurs mainly due to *Staphylococcus aureus, Echerichia coli*, *Pseudomonas aeruginosa*, methicillin-resistant *Staphylococcus aureus* (MRSA). Adequate and proper antibiotic consumption could necessitate and overcome bacterial bloodstream invasion.

**Method:** Our intention was in synthesizing a multipurpose scaffold which could rejuvenate dermal tissues and help in wound care management. We have utilized natural and synthetic material for the preparation of the scaffold.

**Result:** Initially, we prepared dual delivery nanoparticle with a layer by layer assembly which delivers drug to inhibit bacteria in a controlled manner. Vitamin C in the scaffold helps in tissue rejuvenation and the potent drug encapsulated in the nanoparticle releases through diffusion via tiny pores of the scaffolds.

**Conclusion:** Studies suggest that the scaffold is completely biocompatible with very limited toxicity profile and high rate of penetration.

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***Keywords:*** *Bacteremia, Nanoparticles, Scaffold, Biocompatible.*

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**NDDT 02**

# Development, characterization and mechanistic insights of polymeric nanoparticles of gemcitabine

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**Background:** Gemcitabine hydrochloride (GCB), an antitumor agent, inhibits nucleic acid synthesis and is widely explored in treatment of breast cancer, non-small cell lung cancer and pancreatic cancer. Limitations of GCB include high hydrophilicity, low permeability and short half-life. Objective of the study was to prepare polymeric nanoparticles of GCB using Eudragit RS100 for improving its half-life, reduce drug dose and drug stability. Presence of Eudragit RS100 as nanocarrier could be advantageous in targeting to specific site.

**Methods:** Polymeric nanoparticles of GCB were prepared by nanoprecipitation technique. They were characterized for particle size, zeta potential (ZP), drug content, entrapment efficiency (EE) and *in vitro* drug release. Further, nanoparticles were evaluated using SEM, TEM, DSC and FTIR spectroscopy. Mechanistic insights of developed formulation was determined using protein binding study, electrophoretic mobility shift assay (EMSA) and plasma protein binding study.

**Results:** Developed polymeric nanoparticles of GCB showed particle size in range of 200-450nm. Due to physical stability issues, optimized polymeric nanoparticles of GCB were lyophilized and exhibited ZP of +11.9mV, drug content of 96.74%w/v and EE of 68-75%w/v. *In vitro* drug release study results demonstrated sustained release. Protein binding study with BSA revealed protein binding of GCB-loaded polymeric nanoparticles comparable with marketed formulation (Oncogem 200, Cipla Ltd.). In addition to this, human plasma protein binding studies showed negligible interaction of GCB with plasma from both formulations. EMSA study results displayed binding with CT-DNA.

**Conclusion:** Developed GCB-loaded lyophilized polymeric nanoparticles exhibited *in vitro* sustained release. Lyophilized nanoparticles were found to be stable and mecha nistic studies were comparable to that of marketed formulation.

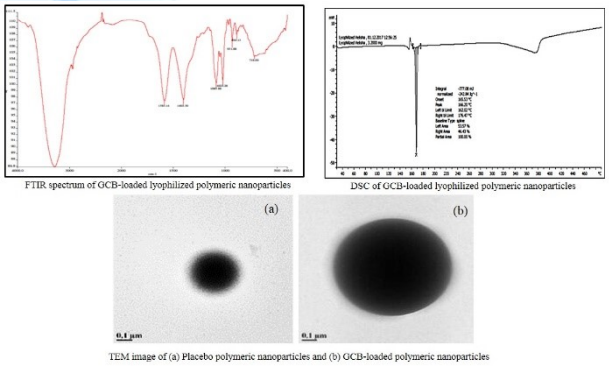


Figure (1): FTIR spectrum, DSC curve and TEM images of GCB-loaded polymeric nanoparticles.

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***Keywords***: *Gemcitabine hydrochloride, Eudragit RS100, nanoparticles, nanoprecipitation*

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**NDDT 03**

# Co-delivery of timolol and hyaluronic acid from semi-circular rings implanted contact lenses for the treatment of glaucoma: *In vitro* and *in vivo* evaluation

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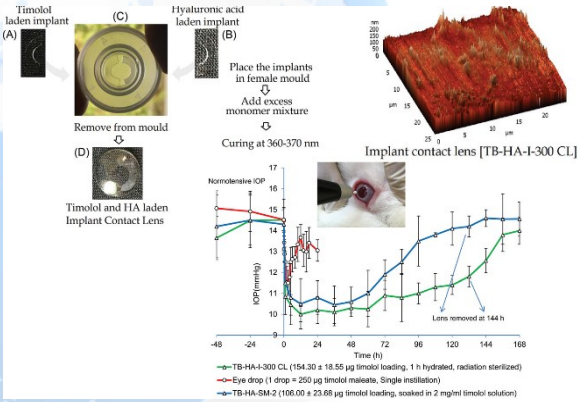
Glaucoma is an ocular disorder caused by increase in intra ocular pressure (IOP) that leads to damage of optic nerve and ultimately causes Blindness. This disease affects around 60.5 million people, leaving 8.4 million with bilateral blindness. And is the second leading cause of blindness worldwide.[1, 2] Majority of the drugs available for ophthalmic conditions are in the form of eye drops and washed off either by tear drainage or by lacrimation, which results in low bioavailability i.e. less than 1-5 %.[3] To sustain the release of ophthalmic drugs, Contact lenses are emerging as a convenient option, but incorporation of formulation changes the optical and physical properties of the contact lenses. Contact lens users have also reported pink eye syndrome, making it unsuitable to be accepted as medical device.

The intent of the present work was to design a novel timolol and hyaluronic acid (comfort agent) loaded semi- circular rings implanted contact lenses that could sustain the release at therapeutic rates without compromising critical lens properties. The drug loaded rings were implanted separately within the periphery of the contact lenses using modified cast moulding technology. The atomic force microscopy report showed an average roughness of 12.38 nm for implanted lens, which was significantly lower in comparison to Freshlook contact lens (116.27 nm). The major amount of timolol was leached (46.47 to 58.79%) during the monomer extraction and moist sterilization (autoclave) steps; therefore the lenses were sterilized by radiation and packaged under dry condition (dehydrated).

The in vitro release data showed sustained release for timolol and hyaluronic acid up to 96 h. The in vivo drug release study on rabbit eyes showed the presence of timolol in tear fluid up to 72 h. The in vivo pharmacodynamics studies showed reduction in IOP till 144 h with low drug loading (154 µg) in comparison to single instillation eye drop solution (250 µg). The study demonstrated the successful application of implantation technology to co-deliver timolol and hyaluronic acid from the contact lenses for extended period of time to treat glaucoma.

**Pictorial Representation**

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***Key words:*** *Timolol, hyaluronic acid, contact lenses, semi-circular ring implants, in vivo release kinetic study, in vivo pharmacodynamic study*

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**NDDT 04**

# Exploring biocompatible thermo-responsive assemblies as antitumor drug delivery systems

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Current tumor therapy facing many challenges due to lack of selectivity and poor solubility of anticancer drugs which causes occurrence of serious side effects. In this work, to obtain enhanced selectivity of anticancer drug uptake by tumor cells the natural ligand hyaluronic acid is grafted with a thermoresponsive polymer. Hyaluronic acid is a biocompatible and biodegradable natural polymer, having high affinity towards CD44 receptors that play significance role in biological function. CD44 receptors get overexpressed in solid tumor cells like pancreatic, breast, lung and these Solid tumors slightly "warmer" than normal cells by considering these fact, we have design selectively targeted temperature responsive anticancer drug carrier hydrogel which can trigger the release of anticancer drug at temperature slightly above physiological temperature approximate at 38°C-39°C.

Thermoresponsive copolymer with LCST 42°C-44°C was prepared by free radical polymerization technique by varying the ratio of thermoresponsive monomer. This polymer was then grafted onto hyaluronic acid to make hybrid polymer with synergistically enhanced characteristics. The final graft polymer was formulated as hydrogel and drug was loaded into it by using a physical mixing method. Doxorubicin (Dox) was used as the model drug for studies. The drug-releasing rate was monitored at 580 nm using UV spectrometer. In-vitro release experiments were carried out at pH 6.5 and pH 6.8 in phosphate buffer at temperature 37°C and 38°C. The structural morphology of these thermoresponsive polymers have been done by using dynamic mechanical analysis, FT-IR, DSC, and GPC.

Hyaluronic acid grafted thermoresponsive polymer was synthesized with LCST 38°C to 39°C. The optimal formulation was composed of 2 mg/mL of Dox and varying concentration (1%, 1.5%, 2%, 2.5%) of hyaluronic acid fabricated thermoresponsive polymer. The release patterns suggested the applicability of developed hyaluronic acid fabricated thermoresponsive drug delivery system to be a target-specific drug platform with great promise for future applications in clinical cancer therapy.

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***Keywords***: *Thermoresponsive biodegradable polymer, biocompatible, hyaluronic acid, CD44, thermoresponsive injectable hydrogel*

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**NDDT 05**

# Investigation of the correlation between the stability of lipidic nanoparticles and polymorphic transitions in the lipid phase

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Polymorphism is the ability to exist in more than one crystalline form due to differences in the lattice arrangements of molecules. Even though the polymorphs are chemically identical, their physical properties can vary significantly. Mostly, the lipids used in the formulation of various lipidic nanoparticles exist in 3 different polymorphic forms as α, β and β' which have close chain arrangement and packing. The process parameters involved in the formulation development and storage conditions of various lipidic nanoparticles can induce polymorphic transitions in the bulk lipid which can severely affect the physical stability of the formulation. It is reported that stabilizers govern the colloidal stability and particle size of lipidic nanocarriers. The objective of this study was to find a suitable stabilizer to modulate the stabilization of lipidic nanoparticles upon polymorphic transition. In the present study VBP1 as a bulk lipid has been selected. In-silico studies were performed to screen the stabilizers wherein the molecular interaction between the lipid and the stabilizer has been studied. A combined approach of DSC and hot stage microscopy was used to investigate the polymorphic transitions. It was observed that 'Gelucire 48/16' and 'Gelucire 50/13' were able to stabilize the polymorphic transitions in the bulk lipid effectively. Hot stage microscopy studies revealed that 'Gelucire 50/13' was able to form a stable nanoparticulate system with VBP1 at room temperature. In this study, the 'in-silico in-vitro correlation' was established successfully to investigate the effect of the polymorphic transitions on the long-term stability of the lipidic nanocarriers.

Table 1: Screening of stabilizers *via in silico* studies

| Sr. No. | Stabilizer | Docking score | DG bind (kcal/mol) |
|---|---|---|---|
| 1 | Tween 20 | -1.903 | -57.7 |
| 2 | Tween 80 | -1.218 | -51.9 |
| 3 | Poloxamer 188 | -0.962 | -25.9 |
| 4 | PVA | -0.794 | -35.1 |
| 5 | Span 80 | -0.835 | -49.0 |
| 6 | Lecithin | -2.173 | -68.1 |
| 7 | Gelucire 48/16 | -3.614 | -118.1 |
| 8 | Gelucire 50/13 | -3.902 | -112.8 |

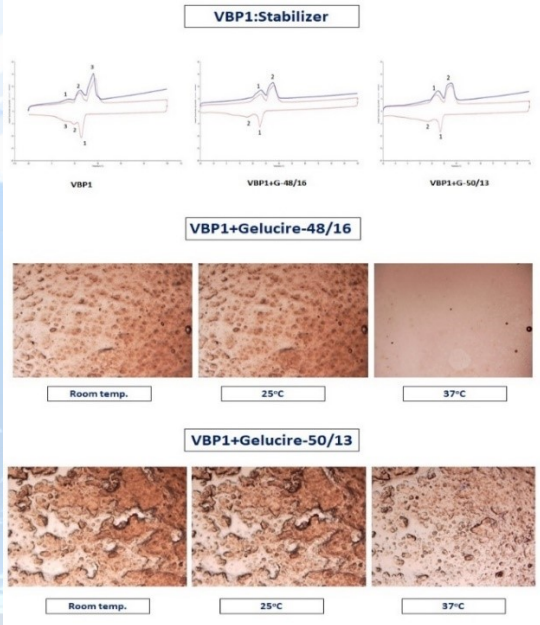


Figure (1): Effect of the stabilizer on the polymorphic transitions in the lipid.

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***Keywords:*** *Solid lipid nanoparticles, DSC, Hot stage microscopy, Polymorphic transitions*

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**NDDT 06**

# Hyaluronic acid nanocapsules enhance chemosensitivity and reduce breast cancer stem-like cells

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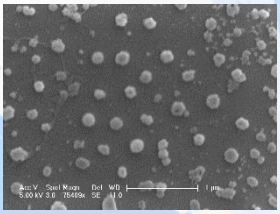
Polyelectrolyte capsules developed using layer-by-layer (LbL) technique have emerged as excellent candidates for drug delivery applications due to their high internal volume, stimuli-responsiveness, and the feasibility to incorporate a wide range of materials as wall components (1). Hyaluronic acid (HA), a mucopolysaccharide found in the extracellular matrix, is responsible for a diverse array of biological functions. The interaction between HA and its receptor CD44 plays a vital role in cancer adhesion, migration, invasion, and growth. Being a negatively charged weak bio-polyelectrolyte, HA can be easily incorporated in LbL assemblies without any covalent modifications. The cellular internalization and targeted drug delivery using HA-based polyelectrolyte assemblies by virtue of the specific CD44 receptor-mediated endocytosis has not yet been well explored.

Herein, polyelectrolyte nanocapsules of HA and protamine were fabricated using LbL technique. These pH- and enzyme-responsive capsules were loaded with an anticancer drug, doxorubicin (Dox). Higher drug release was observed in simulated intracellular conditions like acidic pH and presence of hyaluronidase enzyme. Flow cytometry and microscopy analysis revealed that HA facilitated the targeted delivery and increased Dox concentration in CD44 overexpressed breast cancer cells, MDA-MB-231. Upon internalization via endocytosis, the acidic environment and enzymes in the endocytotic vesicles triggered the encapsulated drug release. However, Dox was effluxed out of the cells much faster in free Dox-treated cells compared to nanocapsules-treated cells. Thus, a slow and sustained release of the encapsulated Dox resulted in the increased chemosensitivity and cell death as confirmed by in vitro cytotoxicity and apoptosis assays.

Further, it is known that the inherently drug resistant cancer stem-like cells (CSCs) that are left behind unscathed after chemotherapy can cause treatment failure and cancer relapse. Increased stemness and over expression of ABC drug transporters as well as epithelial-mesenchymal transition (EMT) genes are all associated with drug resistance in CSCs. In addition, breast CSCs have been reported to exhibit high activity of aldehyde dehydrogenase and overexpression of CD44 (2). Intriguingly, treatment with chemotherapeutic drugs like Dox has also been shown to increase CSCs. Hence, we additionally investigated the effects of HA nanocapsules on breast CSCs. Interestingly, nanocapsule treatment significantly reduced the expression of EMT, stemness, and drug resistance genes as well as the CD44high/CD24low breast CSC subpopulation. Thus, our study highlights the ability of HA nanocapsules to enhance Dox uptake and chemosensitivity and further suggests that treatment with drug loaded HA nanocapsules might reduce therapy-induced stemness, EMT, and drug resistance in breast cancer.

(a)



(b)

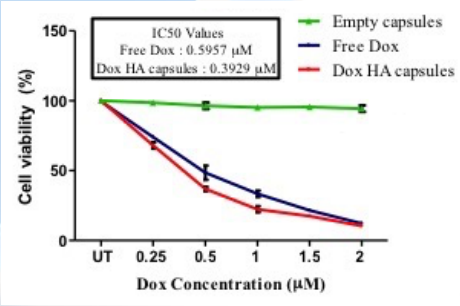



Fig 1: (a) SEM image and (b) MTT assay of HA nanocapsules

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***Keywords***: *Hyaluronic acid, polyelectrolyte nanocapsules, cancer stem cells, drug resistance.*

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**NDDT 07**

# Experimental and *in silico* studies on secondary metabolites from cyanobacterial species with anti-tubercular properties

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Tuberculosis (TB) is a fatal disease caused by Mycobacterium tuberculosis (M.tb) and World Health Organisation (WHO) estimates that one-third of the world population is already infected with M.tb. The rate of incidence is rising by the second and with the emergence of Multiple Drug Resistant Strains. To counteract this problem, there is an urgent need to develop novel anti-mycobacterial drugs from non-conventional sources by using computational biology tool which are active against drug resistant bacteria but, more importantly, kill persistent bacteria.Cyanobacterial extracts are the ultimate source of various types of bioactive compounds with several therapeutic activities like antibacterial, antifungal, anticancer efficacies. These compounds are most effective anti-mycobacterial agent, in comparision to presently used drug. Cyanobacterial compounds belong to the following chemical classes like alkaloids, aromatic compounds, cyclic depsipeptides, cyclic peptides, cyclic undecapeptides, cyclophane, extracellular pigment, fatty acids, linear peptides, lipopeptides, nucleosides, phenols, macrolides, polyketides, polyphenyl ethers, porphinoids and terpenoids. Our study is based on discovery of new anti-mycobacterial compounds through small molecule screening, similarity Search and molecular docking for the prediction of target protein followed by homology modellig. In-silico bioactivity and toxicity class level of these cyano-compounds against M.tb can be analysed. The comprehensive information obtained from this study will help to better understand the structural basis of biological activity of this class of molecules and guide further design of more potent anti-tubercular agents.

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**NDDT 08**

# Design, synthesis and characterization of a dendrimer derived nanomaterial

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**Background**: Dendrimers are highly branched symmetrical nanostructures coming under the class of versatile polymers. Most of the reported dendrimers like poly(amidoamine), poly(propylenimine) have positively charged peripheral groups that hold potential to harm healthy cells by mimicking cationic macromolecules. Such toxic effects can be avoided by building dendrimers using biocompatible monomer units. Hence, our objectives were to design, synthesize and characterize a biocompatible nanomaterial constituting amino acid and fatty acid.

**Method**: Dendrimer derived amphipathic fragment was designed with negatively charged surface carboxyl groups and amide linkages to impart it biocompatibility and biodegradability, respectively. It was synthesized under an inert atmosphere using selected amino acid and coupling reagents. The resulted crude product was purified by column chromatography. The synthesized molecule was analysed using NMR, Mass, DSC, Zeta-sizer and Liquid chromatography studies.

**Results**: Characterization studies confirmed structure and purity of the synthesized molecule. Mass analysis showed m/z of 147.60, 327.75, 866.50, 766.50 and 976.65 for the molecules synthesized at different stages of the designed scheme.

**Conclusion**: A facile method was developed for the synthesis of designed dendrimer derived nanomaterial in good yields. The developed method of synthesis was simple, quick and economical. The designed nanomaterial can be employed therapeutically.

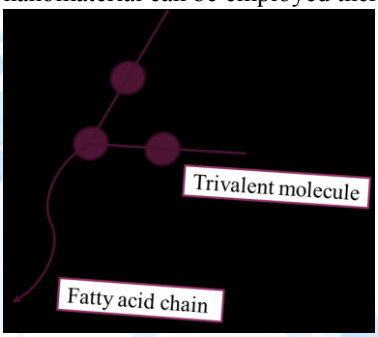


Figure 1: Schematic Representation of Designed Nanomaterial

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***Keywords**: amino acid, amphipathic, biocompatible, dendrimer.*

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**NDDT 09**

# Preparation, characterization and in vitro toxicity study of biodegradable rifampicin nanoparticles

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**Background**: Technological advancement in nanotechnology offering numerous advantages always comes with toxicity and regulatory concerns (1). Polymeric nanoparticles are drawing attention as drug carriers due to their unique advantages such as controlled release, targeting etc. (2). Scientists are concentrating on use of biodegradable polymers as nanocarriers because of accumulation and toxicity concerns related to non-biodegradable polymeric nanoparticles. Albumin, a biocompatible, biodegradable, non-toxic and non-immunogenic protein present in human body can bind to several drugs making it an ideal nanocarrier(3). The present research is mainly focussed on desolvation method and possible toxicological concerns related to the method.

**Methods**: Albumin nanoparticles were prepared by desolvation technique as described previously(3). Different cross-linking tchniques such as glutaraldehyde additiion, UV treatment etc were employed. Also, the impact of different desolvating agents on toxicity profile was analysed using MTT [3-(4,5-Dimethylthiazol-2-Yl)-2,5-Diphenyltetrazolium Bromide] assay.

**Results**: Effect of desolvating agent on particle size of produced nanoparticles was evident from the study. Also, the study suggested that instead of using glutaraldehyde as a cross-linking agent, other methods of cross-linking can produce stable and less toxic nanoparticles by desolvation method.

**Conclusion**: Rifampicin loaded albumin nanoparticles using various cross-linking techniques and different desolvating agents were prepared. Rifampicin loaded nanoparticles with optimized stability, release and toxicity profile will be taken ahead for formulation and in vitro anti-tubercle activity analysis.

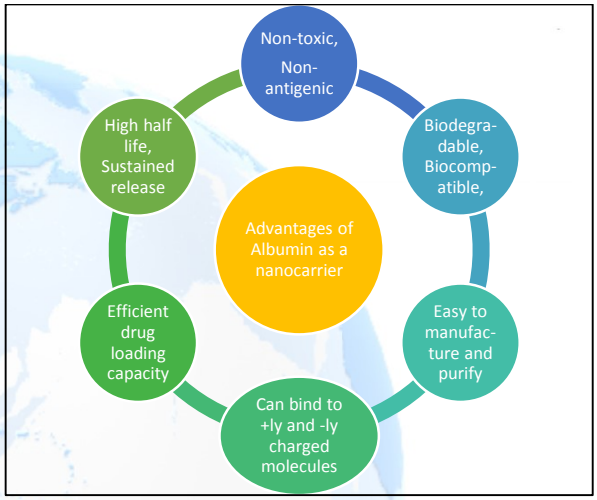


Figure (1)

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***Keywords***: *Nanoparticles, Bovine serum albumin, Nanotoxicity, MTT*

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**NDDT 10**

# Partial amorphization of simvastatin using media milling and spray-drying

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**Background**: High throughput screening and combinatorial chemistry has paved a way for innumberable therapeutically active moieties showing efficacy on life-threatening health ailments.One of the major drawback that prevents development of New Chemical Entities (NCEs) into patient compliant dosage forms is lipophilicity induced poor-solubility. Techniques like solid dispersion, cyclodextrin complexation, etc have been attempted to overcome solubility issues. However, use of excipients and toxic solvents have been found to enhance the formulation complexity and development cost hampering scale-up and marketability. Particle size reduction as a means to enhance solubility and hence dissolution velocity of poorly-soluble drugs has been widely attempted in recent times.[1] The current research work was focussed on exploring a combination of media milling and spray-drying as a means to enhance solubility of poorly-soluble Simvastatin (an antihyperlipidemic) by amorphization.
**Methods**: The stabilizer system (type and concentration) for Simvastatin coarse suspension to be milled was optimized based on contact angle measurement studies. Stabilizers like Sodium lauryl sulphate, Kolliphor ® TPGS (d-alpha tocopheryl polyethylene glycol 1000 succinate), Lutrol F68, Lutrol F127, HPMC E15 and PVPK30 were considered. Duration of high speed homogenisation and ball milling was optimized using particle size analysis. The drug:stabilizer ratio and duration giving lowest size was selected..Simvastatin microsuspension obtained at optimised duration was loaded on carrier and subjected to spray drying.[2,3] Spray-dried micronized Simvastatin was evaluated for morphology by scanning electron microscopy (SEM) studies.The chemical structural details were studied using Shimadzu MIRACLE IR-Affinity 1 FTIR spectrophotometer. The melting characteristics of Spray-dried micronized Simvastatin was studied using Pyris-6 Perkin Elmer Differential Scanning Calorimeter (DSC). Changes in drug crystallinity were evaluated using X-Ray diffraction studies. The in vitro drug release of Spray-dried micronized Simvastatin was studied in phosphate buffer pH 7 containing 0.5% SLS using USP Dissolution Apparatus II (Paddle Type). Solubility of treated and untreated drug was evaluated at 37°C using constant temperature shaker water bath.
**Results**: 0.25% Lutrol F68 in combination with 025% Sodium lauryl sulphate was found to be the optimized stabilizer system for media milling. The coarse suspension with a drug:stabilizer ratio of 2:1 when homogenised for 1 hour followed by 24 hours milling was found to show the lowest particle size. A free-flowing white powder was obtained by spray-drying of the microsuspension. Spray-dried micronized simvastatin was found to exhibit spherical morphology in contrast to untreated Simvastatin which was found to be needle shaped [Fig 1]
**Conclusion**: Media milling in combination with Spray-drying was found to be effective in amorphization of poorly-soluble crystalline Simvastatin resulting in an amorphized Simvastatin with high solubility and drug release characteristics.

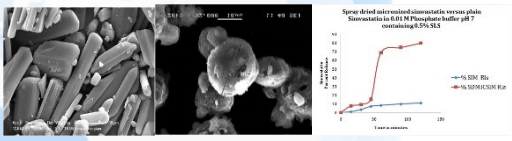

Figure: 1) SEM Images and 2)In vitro drug release of Simvastatin and Spray-dried micronized Simvastatin

No changes in the chemical structure of Simvastatin were confirmed by Infrared spectroscopy studies. Amorphization of Simvastatin was indicated by absence of melting peak for drug in DSC thermogram. Drug amorphization was confirmed by X-Ray diffraction studies by the decrease in intensity of signal peaks. Spray-dried micronized simvastatin was found to show an increase in drug release of 71% as compared to 11% for plain drug.[Fig 2] An increase in solubility was observed for Spray-dried micronized Simvastatin when compared to plain drug.

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***Keywords***: *Amorphization, Simvastatin, poorly-soluble, media milling.*

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**NDDT 11**

# Humic acid alters the physiological and biological properties of titanium dioxide nanoparticles in aquatic ecosystem

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Rapid advancements in applications of nanotechnology have increased nanoparticles emissions in the environment. High reactivity of nanoparticicles due to its small size and large surface area to volume ratio can be diminished because of their homo or hetero-aggregations in the presence of biotic and abiotic factors.1

$TiO_2$ nanoparticles depict organism level toxicity under laboratory conditions, without the influence of either biotic or abiotic factors.2 Among these factors NOM such as humic acid (HA) are known to influence to stability of nanoparticles in the aquatic system due to adsorption on surface of nanoparticles. Therefore, the present study was designed to investigate the potential effect of HA on the stability of TiO2 nanoparticles in different experimental buffers (E3, Dryl's and MilliQ) and their toxicity to a range of aquatic model organisms such as ciliated protozoan (Tetrahymena pyriformis) and early stage embryos of zebrafish (Danio rerio).

It was observed that humic acid increases the dispersion of TiO2 NPs in the experimental buffers by adsorption on the surface of NPs via electrostatic interactions. The maximum aggregation was observed in the E3 medium even in the presence of HA. The intensity of sedimentation of TiO2 NPs was observed in the order: E3 media > Dryl's buffer > MilliQ water. The ecotoxicity results on the Tetrahymena pyriformis and Danio rerio showed that presence of HA reduces the toxicity of TiO2 NPs.

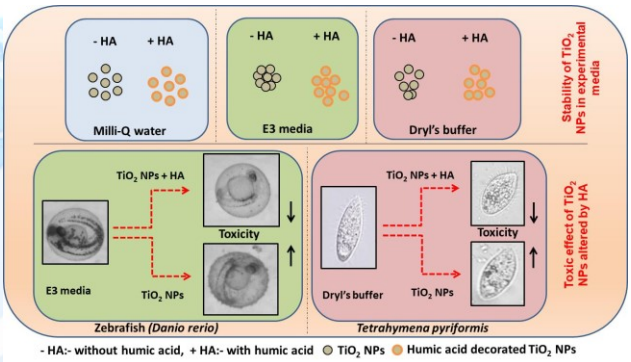


Figure 1: HA reduces the toxicity of $TiO_2$NPs in Tetrahymena pyriformis and Danio rerio.

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NDDT 12

# Anticancer activity of vitamin D encapsulated cinnamon oil nanoemulsion in human alveolar carcinoma cells

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Lung cancer is the most common cancer diagnosed worldwide. In India, lung cancer contributes to 6.9% new cases registered meanwhile causes 9.3% of death every year. Cinnamon oil is used for medicinal purpose since ancient time. Several studies have found that cinnamon oil and active form of vitamin D known as calcitriol, has been shown to possess antitumor activity through inhibiting cell proliferation and inducing cell apoptosis.(1, 2)

Oil-in-water nanoemulsion (NE) of cinnamon oil and vitamin D encapsulated cinnamon oil was formulated using cinnamon oil, vitamin D, nonionic surfactant tween 80 and water by ultrasonication technique. The mean hydrodynamic size of cinnamon oil NE and vitamin D encapsulated cinnamon oil NE was observed as 40.52 and 48.96 nm in complete DMEM F12 media respectively. A concentration dependent increase in the cytotoxic responses of NEs was also observed in A549 cells. The fabricated NEs was inducing DNA damage and micronucleus formation as evident from the comet and CBMN assay indicating their genotoxic response. Both the NEs arrested the cell cycle progression in G0/G1 phase and showed increased expression of Bax, caspase-3 & 9, decreased expression of BcL2 proteins along with significant ($p<0.05$) increase in apoptotic cell population and loss of mitochondrial membrane potential. Thus, both NEs have cytotoxic and genotoxic potential and hence can also be used in food industry as nutraceutical.

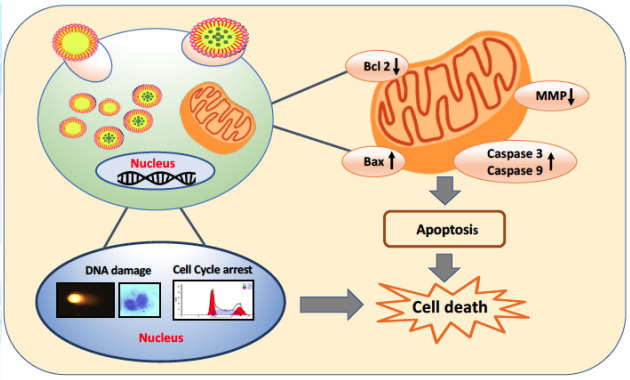


Figure: Schematic Representation of uptake and mode of action of NE in cell.

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***Keywords***: *Nanoemulsion, Ultrasonic emulsification, Cinnamon oil, Vitamin D, Anticancer Activity*

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**NDDT 13**

# Understanding the cellular uptake behaviour of size, shape and surface modified nanoparticles

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The development of nanoparticles (NPs) for a wide range of biomedical applications promises safer and more effective solutions to numerous medical issues. The size, shape, surface charge, and composition of a nanoparticles usually determines the cellular uptake and internalization behaviour. Spherical nanoparticles have been widely used as nanocarriers for delivery of drugs. Nanocarriers are attracting prospective attention due to the realization that non-spherical nanocarriers might exhibit distinctly beneficial effect over spherical ones. Surface modifications of nanoparticles helps in different biomedical applications because surface properties determine the interaction among the components, as well as the solubility and agglomeration behaviour in different solvents. Therefore, understanding the role of nanocarrier in cellular uptake, internalization and delivery efficacy has gained significant interest. Presented here is the i.) PLGA nanoparticles of different size ranges (80-220nm) were studied for the cytotoxicity as well cellular internalization behaviour. ii.) Morphologically, two different shapes such as hollow tubes vs. spherical hydroxyapatite nanoparticles were studied for their biocompatibility as well compared for their dye/drug loading efficiency. iii.) Surface modification of PLGA NPs coated with chitosan were also studied for their cellular internalization. A successful nanocarrier must satisfy a number of design criteria including drug loading capacity, triggered (or appropriate) release, optimized bio-circulation (stealth), serum/plasma stability, nontoxic, targeting, non-immunogenic, cell uptake and non-accumulative. There is a growing recognition that nano-medicine design should learn from natural biological systems, with the realization that nanoparticles formed into nonspherical shapes might exhibit distinctly beneficial properties over similarly sized nanospheres.

## Graphical Abstract

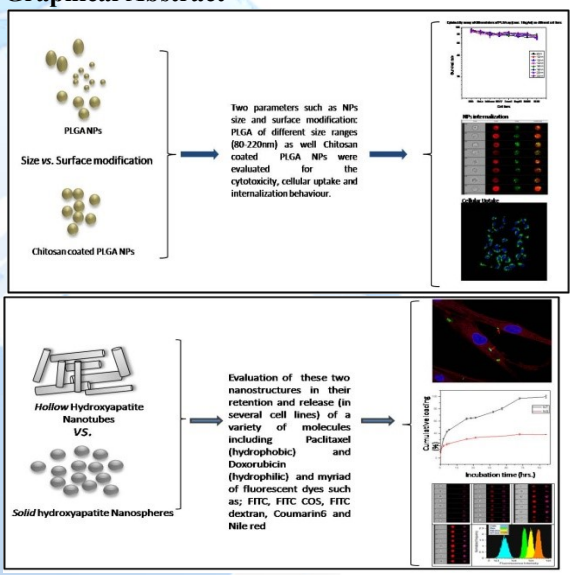


Fig: PLGA NPs size and surface modifications based cellular studies (above), Hydroxyapatite NPs tube vs. spherical shape based cellular uptake studies (below).

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***Keywords***: *Nanoparticles, Morphology, Cell, Internalization, Nanocarriers.*

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**NDDT 14**

# Assessment of in vitro toxicity through MTT assay of biocompatible gold nanoparticles to be used for photothermal therapy (PTT) on different cell line

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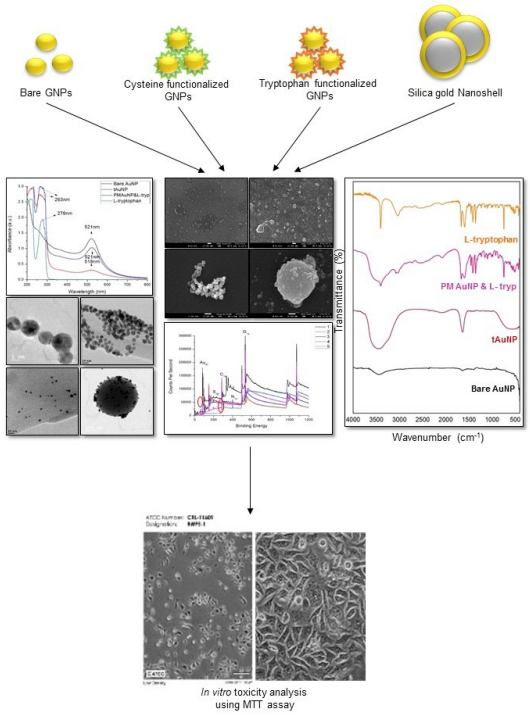
Gold nanoparticle (AuNPs) display unique physical, chemical and optical properties due to their nano dimensions and are used in various biomedical applications like optical imaging, SERS, drug delivery, and photothermal therapy. In vitro toxicity studies of AuNPs showed plausible mechanisms for cytotoxicity like ROS generation, mitochondrial toxicity, cell membrane leakage and apoptosis.1 However, very little is known about toxicity and tissue bioavailability of AuNPs on animals. Also, insufficient data is available which shows changes at molecular level due to toxicity. The OMICS approach can be useful for studying molecular toxicity, and is expected to provide subtle information on the effect of nanomaterials on the living cell.2

Present work is aimed at studying the toxicities of four different AuNP systems with varied functionalization on different cell lines. They are synthesized using chemical reduction method, stober's method and Oldenburg method.3 The characterization techniques like UV-Vis spectrophotometry, FTIR spectroscopy, X-Ray Photoelectron Spectroscopy (XPS), Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) alongwith EDS data for each of these systems showed evidence of their synthesis. These four systems with different sizes are then to be exposed to different cell lines in order to check their dosage toxicity on cells, using MTT assay. This work is under progress currently.

**Graphical Abstract**:

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***Keywords***: *Nanotoxicity, Photothermal therapy, Gold Nanoparticles*

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**NDDT 15**

# Box-behnken design in optimization of ibuprofen ternary solid dispersion

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Solid dispersion technique could serve as a platform to address the issues associated with BCS (Biopharmaceutical Classification System) class II drugs, by increasing their dissolution rate and so oral absorption. The objective of present investigation was to enhance the dissolution rate of ibuprofen by preparing its ternary solid dispersion (SD) using solvent evaporation method. Box-Behnken design was used to scrutinize the combined effect of three independent variables on percentage drug release and flow property of ternary solid dispersion. The independent variables selected were Starcap 1500 (X1), Polyethyleneglycol4000 (X2) and drug: polymer ratio (X3), whereas percentage drug release after 10 minutes (Q10) and angle of repose (AR) were selected as dependent variables. The transformed values of the independent and dependent variables were subjected to multiple regressions analysis to establish full and reduced second order polynomial equations. Using Design of Expert Software, the levels of independent variables was predicted [64.65 % Starcap 1500 (X1 = 1), 10.35 % Polyethylene glycol 4000 (X2 = 0.4) and 25.00 % drug, i.e. 1:3 ratio of ibuprofen: polymer mixture (X3 = 0.50)] for maximized response of Q10 (81.68 ± 4.22 %) with good flow property (angle of repose = 31o63” ± 1o06”). Dissolution profile of optimized ternary solid dispersion was significantly improved in comparison to pure drug. In conclusion, Box-Behnken design demonstrated the application in predicting the values of independent variables for optimization of ibuprofen ternary solid dispersion.

Table: Result for optimized batch for %drug release.

| Batch | X1 (Starcap 1500) | X2 (PEG 4000) | X3 (Ratio of drug: polymer) | **Y1** (Q10± SD) | Predicted | % error |
|---|---|---|---|---|---|---|
| Check pt-1 | -0.3 | -1 | 0 | 65.43 ± 4.06 | 62.88 | 3.89 |
| Check pt-2 | 0.1 | 0 | 0.1 | 73.42 ± 6.06 | 71.16 | 3.07 |
| Check pt-3 | 0.5 | 1 | 0.3 | 88.43 ± 5.26 | 85.06 | 3.81 |
| Optimized batch | 0.92 | 0.76 | 0.93 | **81.68 ± 4.22** | 79.23 | -3.00 |
| Y2(AR± SD) | | | | | | |
| Check pt-1 | -0.3 | -1 | 0 | 40.15 ± 1.06 | 41.57 | -3.53 |
| Check pt-1 | 0.1 | 0 | 0.1 | 36.32 ± 2.06 | 37.69 | -3.77 |
| Check pt-1 | 0.5 | 1 | 0.3 | 37.43 ± 3.06 | 36.49 | 2.51 |
| Optimized batch | 0.92 | 0.76 | 0.93 | **31.63 ± 1.06** | 32.43 | 2.53 |

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***Keywords:*** *Box-Behnken Design, Solid dispersion, Ibuprofen, Starcap 1500, Polyethylene glycol4000.*

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**NDDT 16**

# Elucidation of mechanism of antibacterial activity of microbially synthesized nanoparticles

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The dramatic rise in antibiotic resistance has forced researchers to come up with new strategies to combat drug resistant microorganisms. Silver nanoparticles (SNPs) are of potential interest due to their unique properties and the antimicrobial nature of silver. This study is an attempt to analyze the antibacterial mode of action of green synthesized SNPs.

Culture supernatant of Streptococcus pneumoniae ATCC 49619 was used to synthesize SNPs which were characterized using Fourier Transform Infrared (FTIR) Spectroscopy and Transmission Electron Microscopy (TEM). Minimum Inhibitory Concentration (MIC) of the SNPs was determined against antibiotic resistant *E. coli* and *S. aureus*.

Mode of bactericidal activity of synthesized SNPs was determined. Necrotic cell death was analyzed by assessment of breakdown of plasma membrane. DNA damage was analyzed using DNA fragmentation assay (Fig.1). The activity of glucose-6-phosphate dehydrogenase, which maintains NADPH levels in cells, and hence affects glutathione and oxidative stress levels, was assessed in presence of the SNPs.

Our studies indicate that S. pneumoniae synthesized SNPs have good antibacterial activity against Gram-Positive and Gram-Negative multi-drug resistant (MDR) microorganisms. To the best of our knowledge, this is the first report on elucidation of antibacterial activity of SNPs synthesized using *S. pneumoniae.*

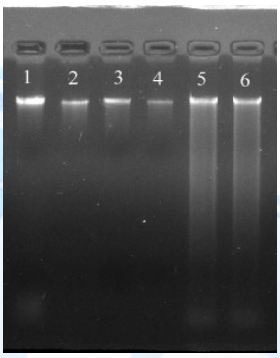


Fig.1: DNA fragmentation assay. Wells 1&2: E.coli control DNA, Wells 3&4: S.aureus control DNA; Well 5: E.coli treated with SNPs; Well 6: S.aureus treated with SNPs.

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***Keywords:*** *Silver nanoparticles, Microbial Synthesis*

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**NDDT 17**

# Green syntheis of silver nanoparticles synthesized from AgNO3 and AgSO4 using *Lumnitzera racemosa* flower buds extract against dengue vector and their eco-toxicity against *Poecilia reticulata*

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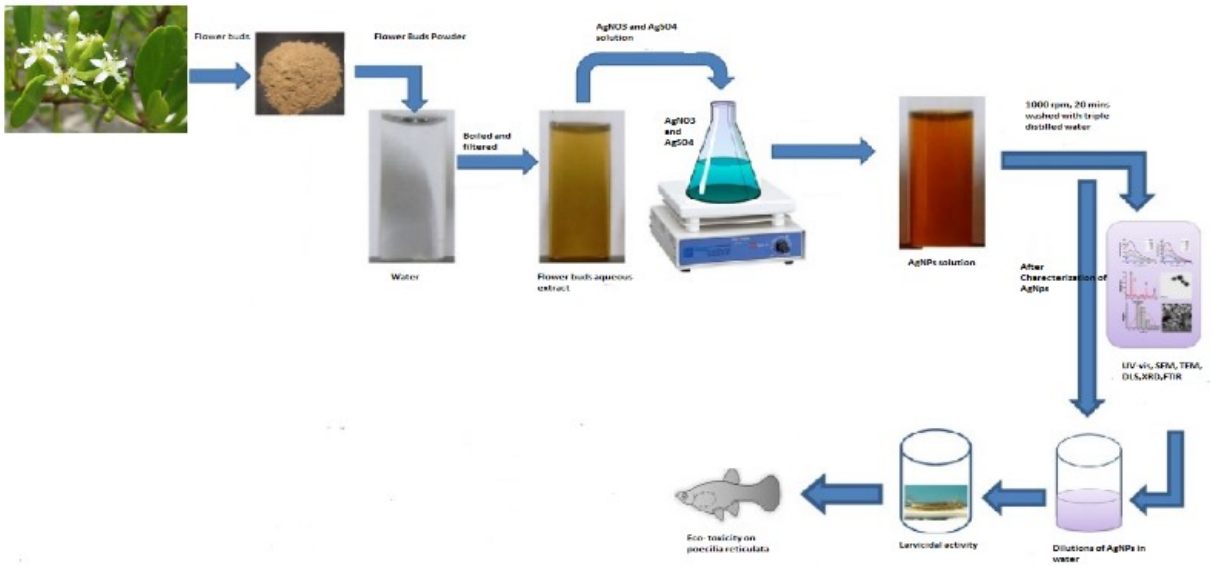
Mosquitoes transmit serious diseases in humans, resulting in millions of deaths each year. Moreover, problems created by using synthetic insecticides include the development of mosquito resistance, environmental pollution and undesirable effects on humans, mammals and other non - target organisms. Insecticides from natural products have gained priority in this area. In the present study, comparative activity of silver nanoparticles (AgNPs) synthesized using two salts AgNO3 and AgSO4 utilizing flower buds aqueous extract from Lumnitzera racemosa, mangrove genus in the family combretaceae was investigated against forth larval instar of dengue vector Aedes aegypti (Diptera: Culicidae). The synthesized AgNPs were characterized by UV-vis spectrum, scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared (FTIR), X-ray diffraction (XRD) and Dyanamic light scattering (DLS). DLS confirmed average particle size (from AgNO3 - 61.59nm, from AgSO4 - 54.09nm). The synthesized AgNPs from AgNO3 and AgSO4 and L. recemosa flower buds aqueous extract were more toxic as compared to crude aqueous extract. The LC50 values were 0.940ug/ml and 0.857ug/ml respectively. The chi-square value were significant at $p < 0.05$ level. Toxicity studies were carried out against non-target fish species poecilia reticulata, most common fish found in the habitats of A. aegypti showed no toxicity at LC50 doses of the AgNPs. These results suggest that the synthesized AgNPs have the potential to be used as an ideal eco-friendly approach to control mosquito vectors. This is the first report on mosquito larvicidal activity of AgNPs synthesized from flower buds of *L. racemosa*.

**Graphical presentation**



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**NDDT 18**

# *In situ* ophthalmic gel of dexamethasone sodium phosphate and chloramphenicol

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**Context:** Poor bioavailability (<10%) of drugs from conventional eye drops is mainly due to the various precorneal loss factors which include rapid tear turnover, systemic drug absorption through naso-lachrymal duct, transient residence time of the drug solution in the cul-de-sac and the relative impermeability of the drugs to corneal epithelial membrane.

**Objective:** The objective of present work was to develop sustain release in situ ophthalmic gel of dexamethasone sodium phosphate (DXM) and chloramphenicol (CHL) using experimental design.

Material and methods: Gellan gum (an ion sensitive polymer) in combination with carbopol 940 (pH sensitive polymer) were used as gelling agent. The developed formulations were characterized for clarity, pH, in vitro gelling capacity, viscosity, assay, in vitro drug release, mucoadhesive strength. Optimum formulation was selected based on validated quadratic polynomial equations developed using response surface methodology.

**Results**: and Discussion: The optimized formulation exhibited 0.2 N mucoadhesive strength; 4013 cps viscosity at physiological condition and 90% release of both drugs over a period of 10-12 hrs.

Conclusion: Mucoadhesive in situ gel for prolong ocular delivery of DXM and CHL was developed using 32 full-factorial experimental design. The developed stable formulation could be a viable alternative to conventional eye drops for treatment of endophtalmitis.

**TABLE:** Results of optimized batch for response variables

| Response variables | Constrains | Predicted value | Experimental value |
|---|---|---|---|
| Y1=Q1% (DXM) | 25≤Y1≥30 | 29.98 | 27.10 |
| Y2=t90% (DXM) | 500 ≤ Y2≥600 | 589.42 | 530.0 |
| Y3=Q1% (CHL) | 15 ≤Y3≥25 | 17.31 | 17.01 |
| Y4=t90%(CHL) | 800 ≤ Y4≥ 900 | 849.72 | 850.0 |
| Y5=Mucoadhesive strength (g) | 15 ≤ Y5 ≥20 | 17.72 | 19.1 |
| Y6=Viscosity at non-physiological condition (cps) | 150 ≤ Y6≥ 200 | 160.35 | 163.5 |
| Y7= Viscosity at physiological condition (cps) | 3500 ≤Y7≥4000 | 3606.43 | 4013 |

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***Keywords:*** *Full factorial Design, response surface methodology, Gellan gum, Dexamethasone sodium phosphate, Chloramphenicol.*

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**NDDT 19**

# Electrochemical method to prepare graphene quantum dots

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Graphene quantum dots (GQDs) are prepared by electrochemical exfoliation of graphite rod. The GQDs have 2–3 nm average size and show excitation dependent Photoluminescence (PL) spectra.

GQDs are 0D graphene nanomaterials with remarkable luminescence properties associated with edge effects.1 As a result, GQDs show great potential towards optical and biological applications etc. GQDs can be synthesized by top-down or bottom-up methods. There is a need of a simple, efficient and affordable method for synthesis of GQDs. In this work, we report a new facile synthesis route to prepare GQDs from graphite rod via electrochemical exfoliation in which the electrolyte used is combination of citric acid and NaOH in Milli-Q water.

TEM show average size of GQDs is 2–3 nm with the size range of 1.5–4.5 nm. XPS spectra show the presence of C=C, C–H, C–O and C=O bonds on the surface of GQDs. The UV-Vis absorption curve show peak at 253 nm corresponds to π→π* transition of sp2 C–C bonds and a shoulder peak at 365 nm correspond to n→π* transition of functional groups present on the surface of GQDs. Excitation dependent PL is observed for GQDs.2

In summary, we have developed a very simple electrochemical strategy to prepare GQDs from graphite rod. Electrolyte used is combination of citric acid and NaOH which makes this strategy green by avoiding the harmful chemicals. GQDs of 2–3 nm with excitation dependent PL makes them a potential candidate for biological applications.

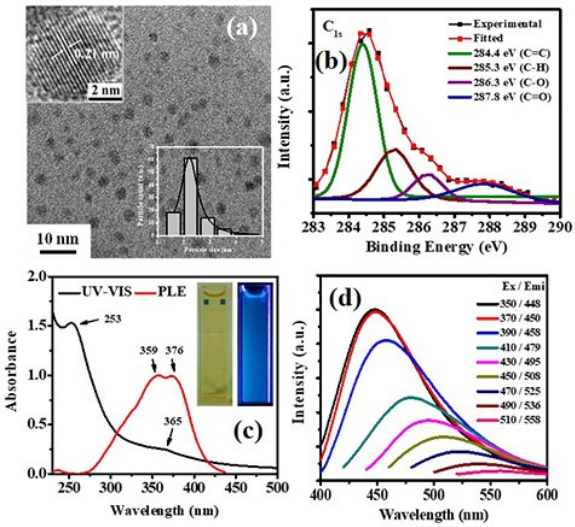


Figure 1: (a) TEM, (b) XPS, (c) UV-Vis and (d) PL of GQDs.

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2. Ahirwar S, Mallick S, Bahadur D. Electrochemical Method to Prepare Graphene Quantum Dots and Graphene Oxide Quantum Dots. ACS Omega 2017;2:8343−8353.

***Keywords***: *graphene quantum dots, electrochemical exfoliation.*

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NDDT 20

# Hydroxyapatite-iron oxide hybrid nanoparticles for hyperthermia and drug delivery applications

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Hydroxyapatite Ca10(PO4)6(OH)2, (HAp) has emerged as one of the most promising material for biomedical applications due to its excellent properties such as biocompatibility, bioactivity, biodegradability, and osteoconductivity etc. Due to its composition similarity with bone and tooth minerals, HAp is extensively used for bone repair and tissue engineering. HAp has also gained increasing interest as a delivery vehicle for carrying various kinds of drugs such as antibiotics, analgesics, anti-inflammatory and anti-cancer drugs. It is well known that hydroxy¬apatite has an excellent bone-bonding ability while magnetic nanoparticles generate sufficient heat to kill tumor cells under an alternating magnetic field. Hence, in recent years, hydroxyapatite - magnetic hybrid nanoparticles have attracted great deal of attention for bone cancer therapy via hyperthermia treatment as well as by chemotherapy of bone tumor.

In the present study, we have synthesized hydroxyapatite-magnetic (HAp-Fe3O4) hybrid nanoparticles with an aim to evaluate their hyperthermia and drug delivery properties. During synthesis, the nanoparticles were functionalized with gelatin moieties in order to give them better dispersibility in aqueous medium. The successful formation of HAp-Fe3O4 nanocomposites is evident from powder X-ray diffraction studies (Fig. 1). The X-ray diffraction peaks corresponding both the phases (HAp and Fe3O4) could be assigned in the PXRD of HAp- Fe3O4 nanoparticles. Fourier transform infra-red spectroscopy also shows the presence of stretching and bending vibrations of HAp and Fe3O4 along with gelatin bands. Dynamic light measurements show that the average hydrodynamic diameter of nanoparticles is ~ 200 nm while the average size of Fe3O4 is ~ 20 nm. This suggests the coating of HAp on Fe3O4 nanoparticles and forming a core-shell structure. The zeta potential of the nanoparticles was found to be ~ 12.0 mV at physiological pH. The nanoparticles were colloidally stable as evaluated by light scattering measurements. The HAp-Fe3O4 nanoparticles generated sufficient heat for killing for tumour cells under an alternating magnetic field (Fig. 2). The presence of negative charge at the surface of nanoparticles provides an opportunity to conjugate positively charged drugs at the surface of nanoparticles. The evaluation of drug loading and release behaviour of these nanoparticles using doxorubicin hydrochloride, an anticancer drug is currently under progress.

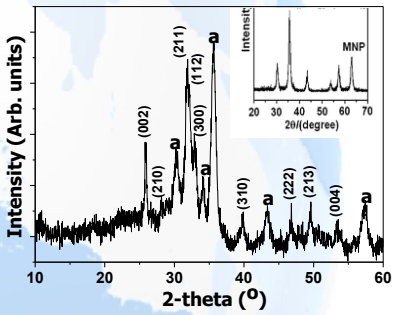


Fig. 1 PXRD pattern of HAp-Fe3O4 hybrid nanoparticles. Inset shows the PXRD of pure Fe3O4. (a corresponds to the peaks belonging to Fe3O4.

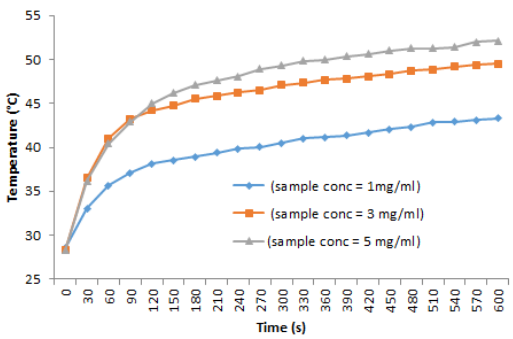


Fig. 2. Temperature kinetic curves obtained after application of an alternating magnetic field (338 Oe) at different concentration of HAp-Fe3O4.

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**NDDT 21**

# Nano-coformulation of docetaxel and pomegranate seed oil for cancer treatment

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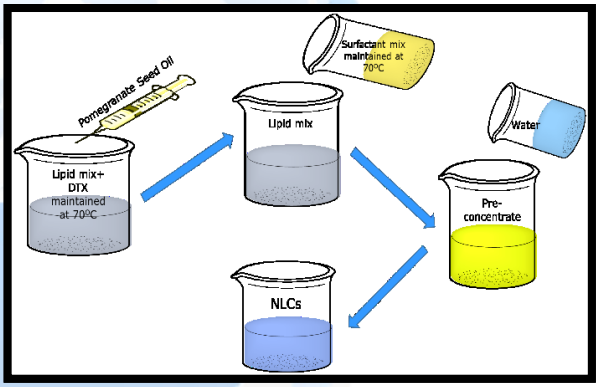
Cancer is the second leading cause of deaths worldwide and accounts for a share of 13 percent in total global deaths. The estimates from Global Burden of Disease (GBD) suggest that about 70 percent of all cancer deaths are now concentrated among low- and middle-income countries. The primary modality of cancer remains surgery; additional radiotherapy, chemotherapy and hormonal therapy comprise other approaches for oncotherapy. However, chemotherapy and radiotherapy lack the specificity needed to kill the cancer cells without affecting the normal cells. In last few decades, lipidic nanocarriers have proven their potential for the effective delivery of various drug molecules. Lipidic systems offer various advantages like biocompatibility, high encapsulation efficiency, potent transfection, lesser toxicity compared to other nanosystems such as polymeric systems. Nanostructured lipid carriers (NLCs) being composed of solid lipid and liquid lipids, offers better stability over other lipidic systems like solid lipid nanoparticles and liposomes.

The current work focuses upon combination delivery of Pomegranate oil and taxol using lipidic nanosystems for chemotherapy of prostate cancer. Docetaxel-pomegranate seed oil-loaded nanostructured lipid carriers (DTX-PSO-NLC) were formulated by melt emulsification method for parenteral delivery. Developed formulation was characterized in terms of particle size, PDI and entrapment efficiency. Optimized formulation was analysed for in-vitro drug release, IR and SEM. The formulation was subjected to stability studies as per ICH guidelines. In vivo pharmacokinetic studies were carried out using male SD rats in comparison with marketed formulation

SEM images depict spherical morphology with a particle size in the range 150-180nm. Around 63-65% of drug was entrapped in the optimized formulation. In-vitro release showed a slow and sustained release of the drug from both the formulation compared to the pure drug.The formulation was found to be stable for a period of 6 months at conditions of 30oC/ 65%RH, 40oC/ 75%RH and 4oC. Pharmacokinetics parameters for all the three formulations were calculated and it was found that DTX-PSO-NLC had better kinetics profile than DTX-NLC and the marketed one.




**Fabrication of DTX-PSO-NLC**

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1. Bharali, Dhruba J., et al. "Nanoparticle delivery of natural products in the prevention and treatment of cancers: current status and future prospects." Cancers 3.4 (2011): 4024-4045.

***Keywords***: *Docetaxxel. Pomoegranate seed oil, NLC, pharmacokinetics.*

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**NDDT 22**

# Liposome of garlic extract: Strategy to prevent and eradicate biofilm in cystic fibrosis

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Cystic fibrosis (CF) is an autosomal recessive disease caused by mutations in the cystic fibrosis transmembrane conductance regulator (CFTR) gene and affects 1 in 2500 newborns worldwide. The primary function of the CFTR protein as an ion channel is the regulation of liquid volume on epithelial surfaces by chloride secretion and inhibition of sodium absorption. In the lung, mutation of CFTR gene results in a decreased mucociliary transport leading to an infection. Most common bacterial infections seen in CF are due to Pseudomonas aeruginosa, Staphylococcus aureus, and Haemophilus influenza. Chronic infection in CF is commonly characterized by the presence of an extracellular polymeric substance (EPS) matrix also referred to as 'biofilm', which presents an entry barrier for drugs. The proposed strategy for CF infections involves the development of a liposome of garlic extract capable of alleviating the symptoms of CF and eradicating the biofilm. Design of Experiments (DoE), a statistical optimization tool based on exploring the relationship between factors affecting the process and process output was used for the optimization of this formulation.

Hence, DPPC and cholesterol containing liposomes were formulated by 'Thin Film Hydration' method. Central Composite Design was used for the optimization of this formulation. Drug: lipid ratio, hydration time, and sonication time were the factors to be optimized with particle size and entrapment efficiency as the studied process outputs. The optimized formulation was further freeze dried and characterized for particle size distribution, zeta potential, entrapment efficiency, and other physical characteristics using DSC, IR spectrometry, XRD and TEM. In-vitro biofilm inhibition assay was also performed.

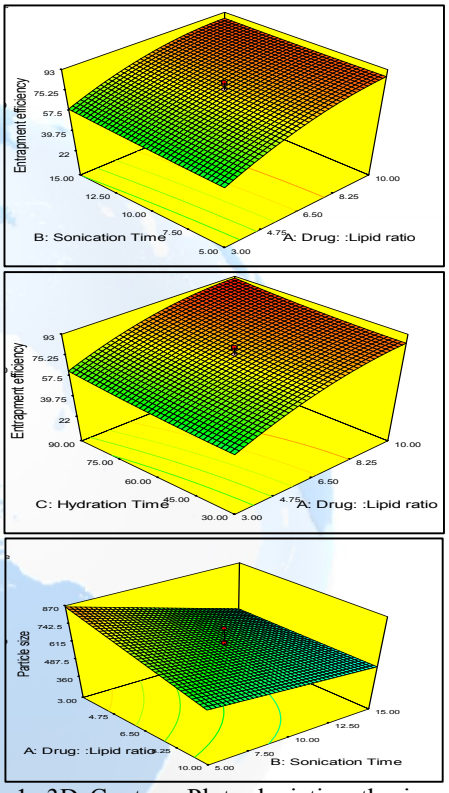


Figure 1: 3D Contour Plots depicting the impact of factors on the responses

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***Keywords*** *Biofilm, Cystic fibrosis, Liposome, Pseudomonas aeruginosa.*

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**NDDT 23**

# Enhancement of biofuel production from microalgae by improving harvesting using iron oxide nanoparticles and increasing the lipid productivity by manipulating the carbon-nitrogen ratio

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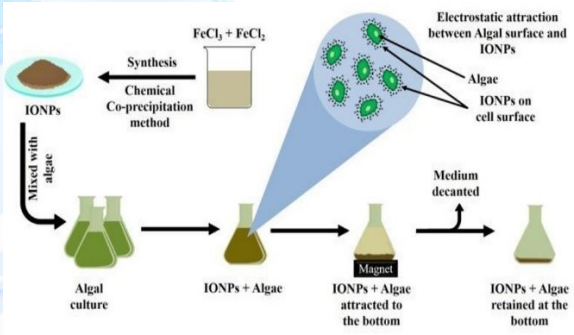
**Background:** Global warming has been on an increase and reducing it with carbon neutral renewable fuels is very important. One of the alternative and sustainable fuel sources of the future is microalgal biofuels (1,2,3). Our study aims to improve harvesting of microalgae using magnetic iron oxide nanoparticles (IONPs) and to increase lipid content by manipulating carbon-nitrogen ratio.
**Methods:** Magnetic iron oxide nanoparticles were synthesized using iron salts by chemical co-precipitation method, characterized by FTIR, XRD, VSM, SEM and Zeta potential. Lipids were extracted by organic solvents and transesterified using sulphuric acid to obtain fatty acid methyl esters (FAMEs) of biodiesel quality.
**Results:** 90% Chlorella pyrenoidosa and 85% Chlorella minutissima was successfully harvested in 60 seconds at a concentration of 500 mg and 600 mg IONPs/L. The harvesting efficiency was due to the electrostatic interactions between charges of the microalgal cell surface and the IONPs. The harvesting of both Chlorella species required less than 60 seconds. The lipid content was maximum when both algae were cultivated in medium deprived of nitrogen and enriched with sodium acetate. The FAME's obtained from such a growth was also maximum with five major types of long chains being present in the methyl esters.
**Conclusion:** Thus, 500 mg/L and 600 mg/L of IONPs harvests 1 L culture medium of Chlorella pyrenoidosa and Chlorella minutissima within 60 seconds; and nitrogen deficiency with excess carbon in the form of sodium acetate gives increased lipid productivity of upto 24% for Chlorella minutissima and upto 23% for Chlorella pyrenoidosa with FAMEs of biodiesel quality.

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***Keywords:*** *microalgae, biofuels, harvesting, lipid extraction*

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**NDDT 24**

# Polycaprolactone based plasmonic nanohybrid for localized photothermal cancer therapy

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Herein, we have developed cost-effective as well as degradable polycaprolactone and chitosan based plasmonic nanoshells for the photothermal cancer therapy.

Gold deposited plasmonic nanoshells are synthesized at ambient conditions by simple reduction employing ascorbic acid. The peak absorption of the gold coated nanoparticles (Au-PCL NPs) has been tuned to NIR region (~740 nm).

These nanoparticles were found to be inert, even at a concentration of 250 µg/ml and didn't show any signs of hemo-toxicity.

The synthesized nanoparticles were found to have photothermal properties and the same was evaluated in-vitro. It was observed that the Au-PCL NPs are capable of destroying cancer cells in-vitro.

These NPs has the potential to destroy tumor cells, irrespective of their nature and resistance status. In addition to the photothermal properties, these NPs could be used as contrast agent.

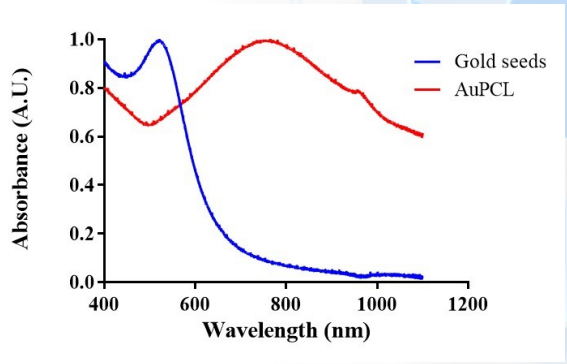


Figure (1): UV-Vis spectra of Au-PCL Nanoparticles

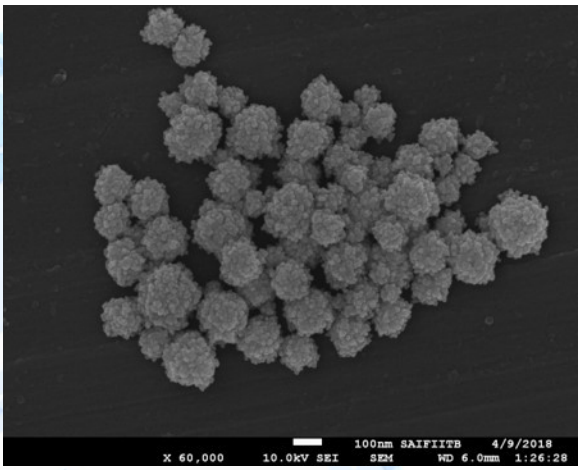


Figure (2): FEG-SEM image of Au-PCL Nanoparticles

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***Keywords***: *PCL: polycaprolactone, FEG-SEM: Field emission gun scanning electron microscope.*

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**NDDT 25**

# Curcumin encapsulated mesoporous silica nanoparticles inhibit pancreatic cancer growth and metastasis potential in animal model

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Conventional therapy regimens for pancreatic cancer (PC) are surgical resection and systemic gemcitabine based chemotherapy. However, the challenges faced in PC treatment are systemic toxicity of gemcitabine treatment, failure in early diagnosis as a prerequisite of surgery, metastasis and chemotherapy resistance. Recently, multiple clinical and preclinical studies have shown that curcumin, a polyphenolic compound, obtained from the medicinal plant turmeric (*Curcuma longa*), is highly effective as an alternative therapy. Thus, in order to solve this problem we explored loading curcumin in Mesoporous Silica Nanoparticles (MSN). MSN is prepared by the sol-gel method and 10% by weight of curcumin was loaded in it. Further curcumin loaded MSN was coated with polyethylene glycol through EDC/NHS linker as well as tumor targeting moiety transferrin attached to the MSN particles. TEM images (Figure-1) reveal uniform, spherical MSN particles of 90-100nm size with well-ordered porous structure (pore size-2.5nm and pore volume-0.62cc/g). The size is further increased to 120-130nm after uniform coating of PEG over the MSN surface. *In vitro* cytotoxicity study in MiaPaca-2 cell show that targeted MSN exhibited 5-folds higher cytotoxicity effect than free curcumin. Further, preclinical imaging study using luciferase reporter labelled MiaPaca-2 cells for developing subcutaneous xenograft model shows that curcumin loaded targeted MSNs can reduce tumor growth significantly ($p=0.0318$). Preclinical results also show dramatic reduction of distant metastasis (Figure-2) to internal organs in curcumin loaded targeted MSN treated mice than free curcumin treated mice. Hence, we propose that curcumin-loaded MSN nano-formulation can be used as an adjuvant to standard medicine for treatment of advanced PC.

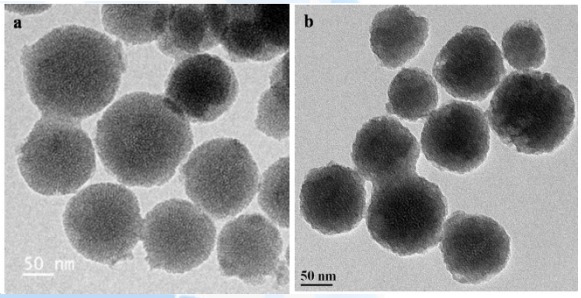


Figure (1): TEM images of a) MSN b) MSN-$NH_2$-CUR-PEG-Tf

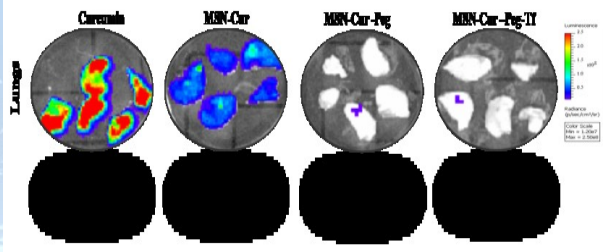


Figure (2): Representative bioluminescence image showing metastasis in lung

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**NDDT 26**

# A mechanistic insight of photothermal therapy potential in treating resistant cancers

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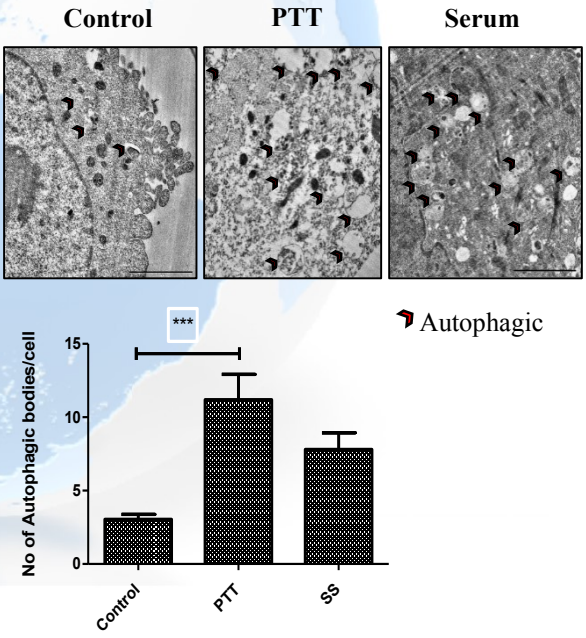
Management of therapy resistant cancer is the prime cause for cancer relapse, which in turn keeps 'Eradicate Cancer' a far-reaching goal. Here we demonstrate gold nanoshell mediated, NIR laser guided photothermal therapy (PTT) as one promising approach for treatment of drug resistant cancer and elucidate the mechanistic basis for PTT mediated cancer ablation. We demonstrate a dramatic response in terms of cell death and reveal that PTT is equally potent ($p<0.001$) in destroying clinically relevant chemoresistant ovarian cancer developed based on A2780 ovarian cancer cell line which can tolerate clinically relevant dose of Cisplatin and Paclitaxel dual treatment. We also show that PTT is equally sensitive to parental sensitive cell, inherently cisplatin resistant SKOV3 cell line or the A2780 based acquired chemoresistant cells *in vitro*. *In vivo* PTT in resistant xenograft mouse model also reveal massive and significant ($p<0.01$) tumor ablation following single laser treatment accompanied with tumor regrowth during follow-up. Hence even if PTT cannot completely cure such aggressive resistant tumors, the overall survival of tumor bearing mice can atleast be doubled which in itself is a significant achievement. Diminished Ki67 and enhanced γH2AX staining in the zone demarcating laser exposed and unexposed tissue area in IHC, establish PTT as a therapy with minimum side effects. Enhanced induction of unfolded protein response pathway and autophagy post PTT is evident from the presence of swollen endoplasmic reticulum (ER) and significant ($p<0.001$) increase in the number of autophagic bodies/cell. The coexistence of swollen ER and autophagic bodies within the same cell coupled with increased protein level of pJNK, show that these two pathways act in concert to mediate photothermal cell death in sensitive and resistant cancers and can even sensitize resistant cancers with inherent high basal level autophagy to a low dose of PTT.



NDDT 27

# Selenium Nanoparticles Encapsulated with Methionine and Folic acid- Reduced Cytotoxicity

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Nanoparticels comprising of semi-conducting cores and encapsulated by biomaterials are promising for application in regulation of Arthritis. Rheumatoid Arthritis (RA) is an autoimmune disorder driven by self-perpetuating free radicals causing extensive bone and cartilage destruction. In this study, we report a facile, multiplex synthesis of a novel nanoparticle functionalized using methionine(Met) and folic acid(Fa). Efficiency of nanoparticles was enhanced by successively layering them with Met and Fa, which increased stability and drastically reduced cytotoxicity. Detailed characterization of the nanoparticles was carried out using UV-spectrophotometry, FT-IR spectroscopy, zeta-potential, X-ray diffraction and ICP-AES. *In vitro* cell viability was studied by MTT assay and dual AO/EB staining using mouse primary cell lines. It is envisioned that the reported Se-NPs coated with Met and Fa will offer a new phase of high-efficiency management of Rheumatoid Arthritis.

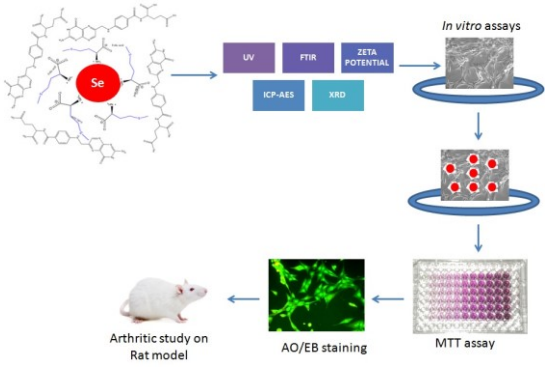


Figure 1: Graphical abstract of SeMetFaNPs and its application in *in vitro* studies.

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***Keywords***: *selenium NPs, methionine, folic acid, rheumatoid arthritis*

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**NDDT 28**

# Unraveling the antibiofilm potential of *Chlamydomonas reinhardtii* sulfated polysaccharides against *Salmonella enterica* and *Vibrio harveyi*

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Nowadays it is known that resistance to antibiotics is often caused by biofilm formation of the microbial pathogen during bacterial infections. The current study aims to investigate the effect of Sulfated polysaccharides (SPs) from *Chlamydomonas reinhardtii* (Cr) on planktonic growth and biofilm forming pathogenic bacteria such as *Salmonella enterica* and *Vibrio harveyi*. *S. enterica* and *V. harveyi* represent a major public health burden worldwide, causing human infections that are responsible for significant morbidity and mortality. While *S. enterica* causes some serious infections like salmonellosis, diarrhoea and many other food borne infections, *V. harveyi* can lead to eye-lesions, gastro-enteritis, vasculitis, and luminous vibriosis. The effect of Cr-SPs on planktonic growth of bacteria was first assessed by zone of inhibition assays which showed prominent clear zones for various extract concentration (0.5mg/ml to 8 mg/ml) against *Salmonella enterica* (16mm to 26 mm) and *Vibrio harveyi* (13 mm to 21 mm). Growth kill activity and reduction in clonogenic propagation further helps us to understand the anti-microbial potential of Cr-SPs against these two bacteria. The extracts showed an inhibitory effect on planktonic growth of Gram-negative *Salmonella enterica* and *Vibrio harveyi* at concentration as low as 440 µg/ml and 490 µg/ml respectively. Antibacterial activity was observed against both bacterial strains with stronger activity against *S. enterica.* Biofilm growth and development were assessed using crystal violet (CV) assays. Cr-SPs inhibited bacteria cell attachment up to 34.65% at 0.5 mg/ml to 100% at 4 mg/ml and 8 mg/ml in *S. enterica* and 40.5% at 0.5 mg/ml to 100% at 4 mg/ml and 8 mg/ml in *V. harveyi.* Biofilm eradication in range of 6.97% to 100% and 28.73% to 100 % was observed over a concentration range of 0.5 mg/ml to 8 mg/ml in *S. enterica* and *V. harveyi* respectively. As quantified by crystal violet method, Cr-SPs significantly decreased biofilm growth in a dose-dependent manner in both these bacteria. Increased reduction in eDNA in the exo-polysaccharide layer with increasing Cr-SPs concentration demonstrated that Cr-SPs specifically interact and destroy the EPS layer formed by biofilm bacteria and there by killing them. The results obtained clearly indicate the Cr-SPs are interesting sources of putative antibiofilm agents. This research can contribute to the development of new strategies to prevent and treat biofilm infections. With further screening and validation of these Cr-SPs, will help to develop them as therapeutic agents against *Salmonella* and *Vibrio* species infections.

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***Key words**: algal sulfated polysaccharides, bacterial infections, anti-biofilm activity, anti-bacterial activity*

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**NDDT 29**

# Development of $Fe_3O_4$ magnetic nanocarriers for anticancer therapeutics

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Magnetic nanoparticles (MNPs) are extensively used in biomedical applications such as drug delivery, tumour destruction via heating (hyperthermia), separation science and MRI diagnosis due to their intrinsic magnetic properties and low toxicity [1]. Nitric oxide has become a promising molecule in the field of chemotherapy [2]. When used along with an anticancer drug, it is shown to have enhanced the effects of the drug. In this respect, we have developed $Fe_3O_4$ MNPs as a carrier for the simultaneous delivery of anticancer drug, doxorubicin hydrochloride (DOX) and nitric oxide.

Citrate functionalized $Fe_3O_4$ MNPs (CMNPs) were synthesized through co-precipitation of ferrous and ferric ions in presence of ammonia as reported elsewhere [3]. The CMNPs were then subjected to the EDC-NHS coupling reaction for co-valent conjugation of cysteine (via amide bond formation between COOH group of citrate and $NH_2$ group of cysteine). The thiol groups on the surface of the Cy-CMNPs were nitrosated using $NaNO_2$ to form NO releasing MNPs. The obtained nitroso modified Cy-CMNPs (SNO-Cy-CMNPs) were then washed using deionized water, separated magnetically and dried at room temperature. Nanoparticles were characterized by various techniques such XRD, TEM, TGA, DLS, VSM, zeta potential, FTIR and UV-visible spectroscopic analysis etc. The anticancer drug, DOX was used as a model drug to estimate the drug loading and release behaviour.

XRD pattern (Figure 1a) of SNO-Cy-CMNPs shows the formation of crystalline single-phase inverse spinel cubic magnetite ($Fe_3O_4$) nanoparticles of average size 10 nm. TEM micrograph of SNO-Cy-CMNPs shows the formation of spherical nanoparticles of size ~10 nm. From HRTEM image, interfringe distance was found to be ~0.30 nm, which corresponds to (220) plane of inverse spinel $Fe_3O_4$. Furthermore, the selected area electron diffraction (SAED) pattern can be indexed to the highly crystalline reflections of $Fe_3O_4$, which is well consistent with XRD results. The successful conjugation of cysteine to CMNPs as well as the conversion of thiol (SH) groups of cysteine to S-nitroso (SNO) was confirmed from FTIR measurements. The absorption band at ~585 $cm^{-1}$ is the stretching mode of Fe-O in $Fe_3O_4$. FTIR spectra of Cy-CMNPs and SNO-Cy-CMNPs showed characteristic bands at around 1612 $cm^{-1}$ and 1400 $cm^{-1}$ and corresponds to the asymmetric and symmetric stretching of $COO^-$. The absorption bands of alkyl stretching vibrations between 2800 and 3000 $cm^{-1}$ are recognized as vibration of functionalized groups of cysteine on the surface of MNPs. Further, the appearance of vibrational modes at 1380 $cm^{-1}$ corresponding to NO groups confirmed the creation of SNO groups on Cy-CMNPs.

The insignificant change in absorbance of aqueous suspension of SNO-Cy-CMNPs as a function of time (even after 24 h) indicates their good aqueous stability. Further, light scattering measurements indicate that SNO-Cy-CMPNs have number average hydrodynamic diameter of 50 nm and possess pH dependent charge conversal features. These nanocarriers also show good magnetic field responsivity under external magnet.

The ability of SNO-Cy-CMNPs as a carrier for delivery of anticancer drug, DOX was investigated using DOX as model drug. The fluorescence intensity of supernatant liquid (obtained after separation of drug loaded particles) decreases upon increasing the concentration of carrier. It has been observed that loading efficiency is strongly dependent on the ratio of carrier to DOX and a maximum drug loading efficiency (w/w) of about 85% is achieved at DOX to SNO-Cy-CMNPs ratio of 1:14.

The pH dependent drug release profile (Figure 1b) of pure DOX and DOX loaded SNO-Cy-CMNPs (DOX-SNO-Cy-CMNPs) were investigated at mild acidic medium (pH 5). While pure DOX shows rapid release behavior (100 % release loaded drug released within 2 h), the DOX-SNO-Cy-CMNPs show sustained release profile at the same pH. The sustained release of DOX from nanocarrier could be attributed to the slow weakening/breaking of the electrostatic

interactions between the drug and the partially neutralized carboxyl groups on the surface of nanocarriers. DOX-SNO-Cy-CMNPs (inset of Figure 1b) shows significant toxicity to the human lung cancer cells (A549), whereas nanocarriers are biocompatible. Specifically, we have developed water-dispersible, biocompatible nanocarrier for anticancer therapeutic applications.

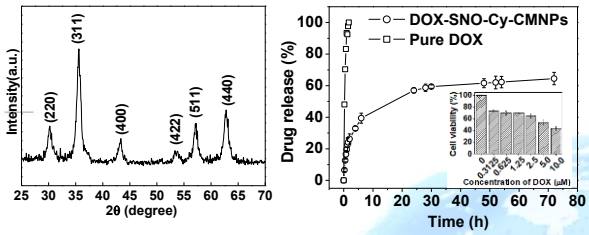


Figure (1): (a) XRD pattern and (b) release profile of DOX from SNO-Cy-CMNPs (inset shows cell viability assay of pure DOX and DOX-SNO-Cy-CMNPs.

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**NDDT 30**

# Nano-particles assisted nested PCR for diagnosis of Malaria

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Malaria is a global scourge that has 220 million cases registered annually out of which there are 6-7 lakh fatalities. Malaria remains to be a completely curable disease if diagnosed early and efficiently. The current techniques used to diagnose malaria are majorly responsible for the mortality and morbidity rate as they lack the sensitivity, especially at the early stages of the disease and are labor intensive. A sensitive, specific, cost-effective and rapid method for malaria diagnosis is need of the hour. The inaccuracy of clinical diagnosis and other conventional diagnosis method increases the urge for proper demonstration of parasitemia prior to therapy. To tackle these important problems there is an obvious need for better implementation of our current methods.

Recently the use of nanoparticles in the field of biological sciences has drastically increased due to their fascinating properties and ability to interact with biomolecules. In this study, we intend to develop an effective and sensitive molecular diagnostic method for Malaria infections using nanoparticle assisted nested PCR. Nested PCR remains the core of malaria diagnosis in research and prevalence studies due to its better sensitivity and able to detect many variable strains of Plasmodium. It consists of primary and secondary reactions. In primary PCR reactions, outer primers can amplify the large conserved region of Plasmodium genus. While secondary PCR reactions include four different inner primers sets for species identification.

The present study compares PCR with and without Gold nanoparticles (AuNP's) for outer primers and multiplex of two inner primers aiming to construct nested-PCR a solidary method in detection and surveillance study of malarial parasites. The positive culture of *Plasmodium falciparum* and *Plasmodium vivax* were obtained from parasite bank of NIMR (ICMR). The DNA from samples was extracted and diluted to process for PCR assay with and without AuNP's. The concentration of AuNP in PCR reaction was optimzed, during which we observed an inhibitory action of the nano particle on polymerase activity with increasing concentration. However, non-specific amplicons were greatly reduce by addition of AuNP in the Nested PCR reaction which further reduced the possiblity of fasle positive results.

The standard size (10nm) AuNP's at optimum concentration (0.25nM) have enhanced the efficiency of target gene amplification through template present in low amount. The amplification for primary PCR reaction has shown increased sensitivity approximately by 5-fold in template sample. The efficient thermal conductivity may be the reason for increased sensitivity. This could prove highly advantageous in early detection and effective in infections with low parasitemia through nested PCR and may be potent in employing in surveillance investigation.

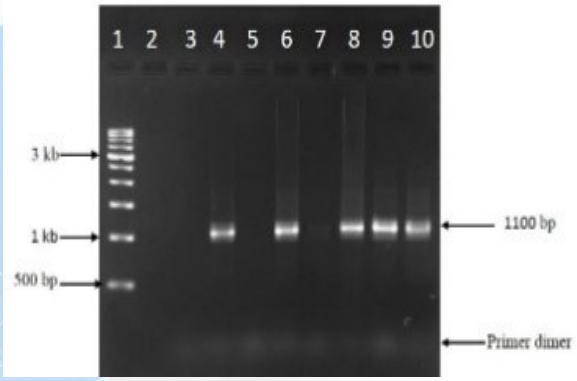


Figure (1): Template Gradient with and without (w/o) AuNPs (0.25nM). Lane1: 500bp DNA Ladder; Lane2: Non-Template Control; Lane3: 12.55ng template w/o AuNP; Lane4: 12.55ng template with AuNP; Lane5: 25.1ng template w/o AuNP; Lane 6: 25.1ng template with AuNP; Lane 7: 37.65ng template w/o AuNP; Lane8: 37.65ng template with AuNP, Lane9: 50.2ng template w/o AuNP; Lane 10: 50.2ng template with AuNP.

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***Keywords:*** *Nano-PCR, malaria, diagnosis*

**NDDT 31**

## Identification of new world antibiotic (ENZYBIOTIC) from *Periplaneta americana*

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Proteins are basic structural and functional unit of cell which perform multiple functions like defence, catalytic, hormonal, transport etc. Proteins as catalyst are known to act specific for their substrate. However, many enzymatic proteins are explored to have multiple catalytic activities. The study undertaken has unveiled such proteins which play important role in insect metabolic activity as well as defence mechanism against pathogenic bacteria. Out of seven proteins bands isolated from *Periplaneta americana* brain lysate, two protein bands were considered for identification using MALDI-TOF MS/MS. The antibiotic assays of these protein elutes indicated effective control on bacterias like *MRSA, S.typhi, S.paratyhi, P. aeruginosa*. The proteins were identified as Transferrin (79.91 kDa) and Glyceraldehyde-3-phosphate dehydrogenase (35.58 kDa). Earlier studies on enzymes such as GA3PDH indicated antimicrobial characteristics in human placenta and antifungal activity against *Candida albicans* (Jeanette W. et.al.). Iron binding protein, Transferrin, isolated from *Bombyx mori* is found to have antimicrobial activity against several gram positive and gram negative bacteria. In future "enzybiotics" could be the possible sources for the treatment of drug resistant bacterial infections. Sequence similarities of Enzymes such as GA3PDH can be considered in the development and as potent sources for vaccines used against bacterial infections in aquaculture.

***Keywords:*** *proteins, moonlightening, enzybiotic, MALDI-TOF MS/MS, drug resistant bacteria*

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**NDDT 32**

# Effect of counterions on the conformational changes of protein upon interaction with magnetic hydroxyapatite nanoparticles

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Recent development in nano-biotechnology shows that protein–nanoparticle (P-NP) interactions determine the behaviours of NPs in the surrounding bio-systems. As NPs enter biological fluids, proteins and other biomolecules such as lipids adsorb to their surfaces with various exchange rates leading to the formation of the biomolecular corona.[1] The adsorption on NPs influences the structure and bioactivity of proteins which further dictates the fate of NPs in the biological environment.[2] Hence in depth understanding of the factors governing the protein –NP interaction is essential.

Hydroxyapatite (HAp; $Ca_{10}(PO_4)_6(OH)_2$, stoichiometric Ca/P molar ratio 1.67), a major component of bones and teeth, have emerged as a new class of biomaterials due to its outstanding biological properties such as non-toxicity, biocompatibility, lack of inflammatory response and absence of immunological reactions.[3] Recent reports have shown that the combined effect of magnetite and hydroxyapatite nanostructures provide efficient means for diagnostic and therapeutic applications which can be controlled with an external magnetic field.[4] For these applications an important aspect to be considered is the interaction of the magnetic hydroxyapatite (MHAp NPs) with biomolecules such as protein (P) and their biological response.

The present study focusses on the synthesis and characterization of MHAp-NPs that exhibits excellent biocompatibility, making it an ideal candidate as a biomaterial. The interaction of MHAp NPs with proteins was investigated with and without surface functionalization of the MHAp NPs. The MHAp NPs were surface functionalized with tri-lithium citrate and cetyl pyridinium chloride having $Li^+$ and $Cl^-$ as counter-ions, respectively. Hen egg white lysozyme (HEWL) and pepsin A were used as positively and negatively charged model proteins respectively. The P-NP interaction was characterized by Zeta-potential measurements, UV-visible absorption and fluorescence emission spectroscopy. The secondary structure of the protein was investigated using circular dichroism spectroscopy. The functionality of the interacted protein upon interaction with and without surface functionalized MHAp NPs was studied using enzyme activity assays.

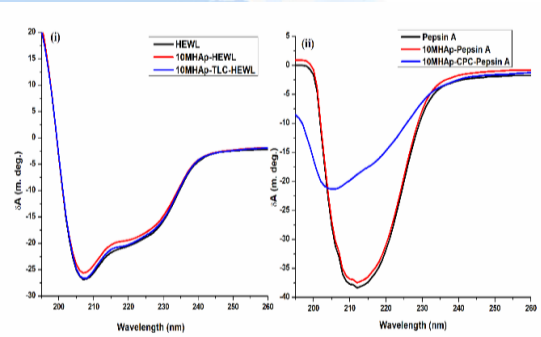


Figure 1: CD spectra of the secondary conformations of (i) HEWL and (ii) pepsin A with and without surface functionalized MHAp NPs

Figure 1 shows the CD spectra of the proteins upon interaction with MHAp NPs. Each spectrum was deconvoluted using the CDNN2.1 software and protein secondary conformations were measured. The interaction of HEWL with unfunctionalized MHAp did not show any major change in the CD spectra indicating no significant unfolding of HEWL whereas TLC functionalized MHAp showed a minor effect on the secondary structure of HEWL (Fig 1 (i)). A significant change in the CD spectra was noted in the CPC functionalized MHAp NPs upon interaction with pepsin A as compared to that of the native protein (Fig 1 (ii)). It has been reported earlier that HEWL binds electrostatically with TLC functionalized spherical iron oxide nanoparticles, wherein the associated counterions ($Li^+$), diffused into the bound proteins and irreversibly unfolded them, and the interaction was

named as the 'reverse charge parity counterions' or RCPC interaction. [5] However in this present study no conformational changes of HEWL was noticed which was attributed to the negative surface charge of MHAp NPs. The $Li^+$ ions were immobilized into MHAp NPs and hence their availability for diffusion into the protein was reduced. In case of CPC functionalized MHAp NPs, the $Cl^-$ counterion of CPC will have a higher tendency to diffuse away from the negatively charged functional groups of MHAp NPs thereby contributing towards the significant unfolding of Pepsin A. The counter ions thus unfolded the protein structure. The Enzyme activity assays were in accordance with the CD data which verified the functionality of the interacted protein.

The size and the charge of counter-ions associated with the functionalized NPs thus play a vital role in the unfolding of the protein structure. In depth understanding of the P-NP interaction is thus crucial for upcoming biomedical applications.

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***Keywords:*** *magnetic hydroxyapatite nanoparticles, P-NP interaction, counter-ions and conformational changes*

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NDDT 33

# Synthesis and biological evaluation of new thiazolyl-2-amine schiff base derivatives as potent antitubercular agent

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**Background:** The frequency of infectious disease like tuberculosis in humans has increased dramatically because of rising multidrug resistance. The rising clinical importance of drug-resistant bacterial pathogens has impelled additional exigency to investigate formore effective agents.Recently it is reported that thiazole based compounds demonstrated considerable potential as anti-tuberculosis (I, II), Antimicrobial (III, IV), Anticancer (V) and Antibacterial (VI) agents (Fig. 1) [1-5].

**Methods:** A series of some new thiazolyl-2-amine based Schiff base derivatives (4a-4f) have been synthesized by a reaction of 3-[2-amino-4-(4-bromophenyl)thiazol-5-yl]chromen-2-one (2) with various aldehyde derivatives (3a-3f). The newly synthesized Schiff base derivatives were characterized by FTIR, $^{1}$H-NMR, $^{13}$C-NMR and Mass spectrometry. All the Schiff base derivatives were screened *in vitro* for their antibacterial activity against *Mycobacterium tuberculosis* (H37 RV strain) ATCC No-27294.

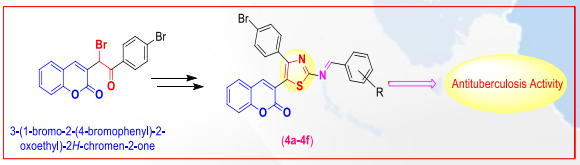


Figure (1): Scheme of preparation.

**Result:** Among the compounds tested, compounds 4c and 4f showed potent antitubercular activity against *M. Tuberculosis* at MIC 6.25 µg/mL.

**Conclusion:** In this work, we studied the synthesis of Schiff bases (4a-4f) by condensation reaction of 3-[2-amino-4-(4-bromophenyl)thiazol-5-yl] chromen-2-one (2) and benzaldehyde derivatives (3a-3f) (Fig. 2). The spectral characterization supported structures of all Schiff bases (4a-4f) represented in Table 1. Antitubercular screening of all the synthesized compounds shows some compounds exhibit excellent antitubercular activity against M. tuberculosis (H37 RV). These outcomes are worth further investigation.

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***Keywords:*** thiazole, coumarin, Schiff base, heterocycle, tuberculosis.

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**NDDT 34**

# Nanocrystalline tin oxide thin film based biosensor for detection of antigen-antibody complexes

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Biosensors are small analytical devices used for the detection of a specific analyte (enzymes, virus, bacteria, cells and DNA) in a rapid and cost effective manner. It combines a biological component with a physiochemical detector. The present study describes fabrication and characterization of Tin oxide thin film based electrochemical sensor for label free, cost effective detection of antigen-antibody complex.

Nanocrystalline $SnO_2$ thin film was prepared on p-type silicon substrate using Langmuir Blodgett technique. $SnO_2$ film surface was functionalized by electrochemically depositing Polyaniline (PANI) film for biomolecule immobilization. Antibody (Ab) molecules (mouse IgG) were immobilized through glutaraldehyde coupler [1]. Electrochemical cell consisted of antibody immobilized $Si/SnO_2$ thin film as working electrode, platinum plate and wire as counter and pseudo reference electrodes, phosphate buffered saline (PBS, PH 7.2) as electrolyte. Potentiostat/Galvanostat PGSTAT20, Echochemie, the Netherlands, was used for cyclic voltammetry and Capacitance-Voltage measurements. For detection of antigen-antibody interaction the corresponding specific antigen (An), goat antimouse IgG from whole serum was used. Reusability of the sensor was tested by treating the substrate with 3 M KCl for 150s to remove the bound antigen.

Cyclic voltammetric experiments showed an effective current changes after each process step namely, PANI deposition, Ab immobilization and An interaction (Fig. 1). After each process step, the capacitance (Fig.2) changes at positive applied bias voltage. Capacitance decrease after antigen (1.4 µg/ml) injection indicating Ab-An interaction. Both cyclic voltammetric and capacitance voltage plots indicate the specific interaction of antigen with immobilized antibody.

Specific binding of Ab with An involves hydrogen bonding and electrostatic interactions which in turn will affect the electrode/electrolyte interfacial properties. Further studies are being carried to study effect of possible micro interfacial pH variations at the electrode/electrolyte interface due to specific Ab-An binding.

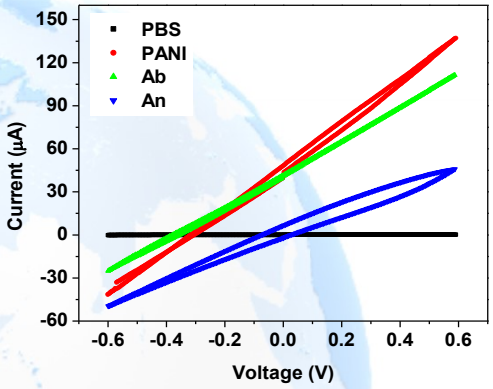


Figure (1): Cyclic Voltammetry plot recorded at 50 mV/s scan rate, after each process step.

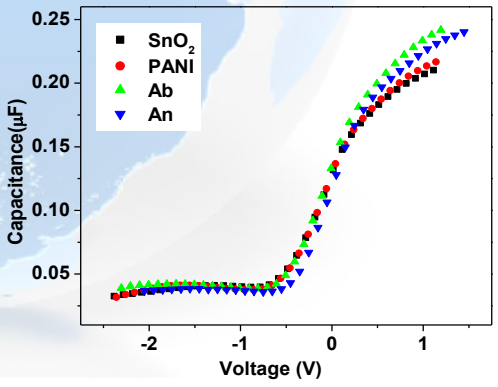


Figure (2): Capacitance vs. Voltage plot recorded at 1 kHz, after each process step.

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**NDDT 35**

# Development of endometroid adenocarcinomas in mice: Role of HOXA10

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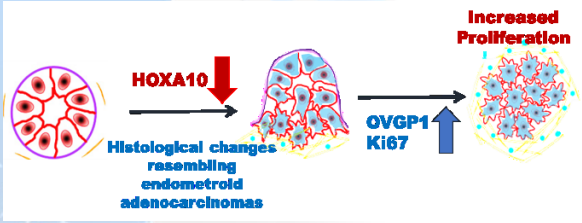
Amongst, all the gynaecological malignancy, endometrial adenocarcinomas accounts for 4.8% cancers in women globally. Various mouse models have been used, where alterations in two or more genes have led to development of endometrial adenocarcinomas, suggesting combinatorial effect of the genes. Among the several genes implicated in endometrial cancer, we have investigated the role of HomeoboxA10 (HOXA10), a transcription factor, which is a member of AbdB cluster of HOXA genes family. HOXA10 is required for specification specifies uterus during embryogenesis and is it is required for embryo implantation in adults. In the present study, we performed integrative transcriptomic analysis using GEO datasets in women with endometrial adenocarcinomas, where decrease in levels of HOXA10 in the uteri of women with endometrial cancer. To further envisage the role of HOXA10 in endometrial cancer, we generated mice knockdown for HOXA10 expression (HOXA10 hypomorphic mice). On histological examination of the uteri of hypomorphs, revealed development of features resembling endometrial hyperplasia and endometroid adenocarcinomas, which included features like glandular crowding, cribriform structures, intraglandular bridges without intervening stroma, extensive papillary structures, and villoglandular structures. The uteri of the HOXA10 hypomorphs were highly proliferative as indicated by Ki67 staining. he morphological feature observed in hypomorphs were also paralleled by the molecular changes i.e. gain of oviductal glycoprotein (OVGP1) and aberrant expression of ER alpha and beta. Normal endometrium does not express OVGP1, and gain of OVGP1 is specific to endometrial adenocarcinomas, we investigated the role and regulation of OVGP1 in endometrial adenocarcinomas. For this, OVGP1 expression was knockdown in Ishikawa cells and results revealed, loss of OVGP1 reduces cell proliferation and enhances homotypic adhesion via E-cadherin. ***ConTra v3*** analysis revealed HOXA10 binding elements on OVGP1 promoter. Integrative transcriptomic analysis reveal HOXA10 and OVGP1 are inversely correlated. In summary, our findings demonstrate that the mere loss of *HOXA10* in mice is sufficient for the development of features resembling well-differentiated adenocarcinomas in humans, which are positive for *OVGP1* expression.

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**NDDT 36**

# Development of pH sensitive tablet for colon drug delivery using chemically modified Guar gum co-polymer

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In recent years, considerable attention has been focused on use of natural hydrophilic polysaccharides for tablet formulation, because of their flexibility, easy availability and to obtain a desirable drug release profile, cost-effectiveness and broad regulatory acceptance. These modified polysaccharide have the common properties of polysaccharides including compatibility, biodegradability and higher thermal and shear stability.

**Aim:** The purpose of this study was to prepare pH-sensitive tablet using an polyacrylamide and Hydrolyzed grafted guar gum.

**Method:** Polyacrylamide-grafted-guar gum (pAAm-*g*-GG) was prepared by taking three different ratios of guar gum to acrylamide (1 : 2, 1 : 3.5 and 1 : 5) using microwave irradiation technique. Among these optimized batch of polyacrylamide grafted guar gum were was converted to hydrolyzed Guar gum by saponification. Amide groups of these grafted copolymers were converted into carboxylic functional groups. Fourier transform infrared (FT-IR) spectroscopy, Differential Scanning Calorimetry (DSC) and $^{1}$H-NMR spectroscopy were used to characterize the grafted and hydrolyzed copolymers. Tablets were prepared by pAAm-*g*-GG (1.0–4.5%) and microcrystalline cellulose incorporating an antibiotic *viz.*, Cefixime. Here, variables were studied and tablets were characterized for average size, surface morphology, friability, bulk density and flow properties. Swelling index was carried out in simulated gastric and intestinal conditions.*In vitro* drug release was carried out in simulated gastric and intestinal conditions.

**Result:** The *in vitro* drug release profile indicated an increase in drug release retardation with increasing pAAm-*g*-GG concentration. The formulated tablets were stable with respect to their physicochemical characters and drug content over a period of 12hr at room temperatures and relative humidity.

**Conclusion:** It has been concluded that the prepared tablets demonstrate the potential use of MCC and pAAm-*g*-GG for the development of pH sensitive colon specific controlled drug delivery systems of Cefixime for various antibiotic drug delivery.

**Summary:** The optimized formulation from grafted guar gum tablet was compared with hydrolyzed grafted guar gum tablet and plain guar gum tablet,the hydrolyzed grafted guar gum tablet formulation exhibited excellent pH dependent drug release up to 11 hrs.

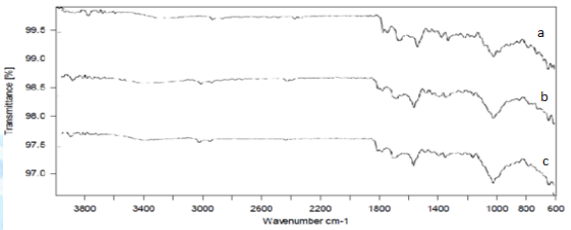


Figure (1): FTIR of (a) Guar gum, (b) polyacrylamide guar gum & (c) Hydrolyzed Guar gum.

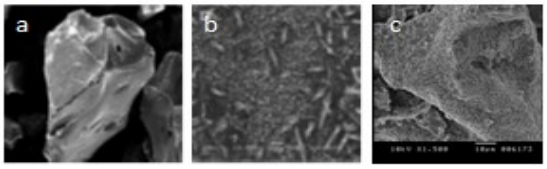


Figure (2): SEM of (a) Guar gum, (b) polyacrylamide guar gum & (c) Hydrolyzed Guar gum.

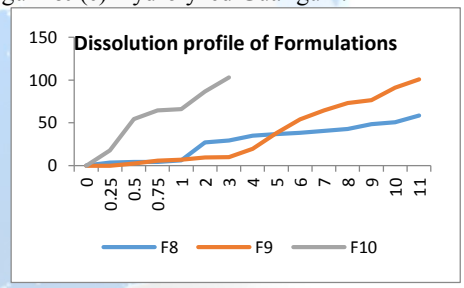


Figure (3): Dissolution Profile of Gaur gum (F8), Polyacrylamide Guar gum (F9), Hydrolyzed Guar gum (F10)

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***Keywords:*** *hydrolyzed Guar gum, grafting, polyacrylamide, microwave, cefixime*

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**NDDT 37**

# Encapsulation of bioactives on magnetite nanoparticles: A targeted drug delivery approach

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Plant bioactives having antioxidant & medicinal properties are being targeted for treatment of cancer and various diseases and their market is increasing rapidly in a highly polluting environment. Most of the plant bioactives are hydrophobic in nature, having high rate of metabolism and rapid systemic clearance, thus resulting in their poor bioavailability and lower therapeutic efficacy. Nanoparticles when conjugated with plant bioactives exhibit increased bioavailability and enhanced pharmacological activity.[1] Magnetite nanoparticles represent unique class of drug delivery vehicles due to their magnetic behaviour and thus have potential use in biomedicine. The surface area of Magnetite NPs can be modified & functionalised by attachment of various plant bioactives.[2,3] The present study proposes encapsulation of plant bioactives on green synthesised magnetite nanoparticles via self assembly methods. Plant bioactives used were Essential Oils having powerful antioxidant properties. Techniques used for confirming the formation of the conjugates were XRD, FTIR, VSM, SEM, TEM and DLS methods. Drug entrapment efficiency, antioxidant assay & antibacterial activity were evaluated and showed promising results. Thus integration of nanotechnology and plant bioactives can open up new era in therapeutics and targeted drug delivery.

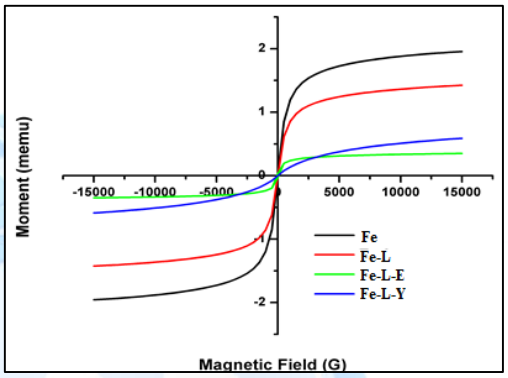


Figure (1): Magnetisation study of as synthesised hybrid magnetite nanostructures

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***Keywords***: *Magnetite, Green Synthesis, Bioactives, Antioxidant Activity.*

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**AMC 01**

# Thermal degradation study of some commercial nuclaer and non-nuclear grade resins

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The thermal degradation study of nuclear grade polystyrene sulfonic cationites, Tulsion T-46, Indion-223 and non-nuclear grade polyacrylic carboxylic cationite, Indion-236 was carried out using thermogravimetric method to understand the probable degradation steps. In order to further investigate the decomposition steps, Scanning Electron Microscopy (SEM) was used in addition to thermal analysis. The TGA results shows that Indion 236 resins shows the total weight loss of 88.58 % up to 530°C of which 10.57 % mass loss was observed up to 200°C. The second mass-loss step between ~210 and ~390 °C can be assigned to polyanhydrides decomposition processes. The last decomposition step between ~400 and ~530°C corresponds to the total degradation of the polymeric matrix and of the depolymerization fragments. Tulsion T-46 shows total weight loss of 55.12 % up to 530°C, of which ~ 32.14 % weight loss take place up to 200°C. The major weight loss starts in the temperature range of 280–400°C which is mainly due to the volatilization of degradation products. TGA curve of Indion – 223 shows total weight loss of 61.61 % up to 520 oC, of which ~ 29.80 % weight loss take place up to 200 °C. The second weight loss begins at 270 °C and ends at 400 °C, due to slow degradation of side chain and loss of sulphonic functional group. The mass loss from 400 °C to 520 °C was gradual which might be due to degradation of styrene/DVB matrix. The SEM pictures of Indion-236 resin polymer exhibits dent on the surface at 400°C. In case of Tulsion T-46 resin complete cracking of the spherical structure was observed. The surface morphology of Indion – 223 at 400° C shows crack in the spherical structure which supports breaking of polymer matrix at that temperature.

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**AMC 02**

# Designing nanostructured tungsten trioxide for improved electro-capacitive performance

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Tailored nanostructured materials have a critical role for addressing the present challenges in energy, environment and health sectors. Nanostructured tungsten oxide (WO3) is one such versatile material that has found promising applications in the above mentioned sectors.1-3 This work describes the use of a modified sol gel method to design WO3 nanostructures without the need of any expensive templates or hydro/solvothermal conditions. The synthesized WO3 nanostructures are characterized for their phase purity, size, shape and morphology using various surface characterization techniques. H+ intercalation efficiency and diffusion coefficient of nanostructured WO3 were investigated using cyclic voltammetry.4,5 Galvanostatic charge discharge studies were also performed to show the improved electro-capacitive performance of nanostructured WO3. The simplicity of our synthesis method to produce nanostructured WO3 with enhanced electro-capacitive performance demonstrates promising results for device scale applications.

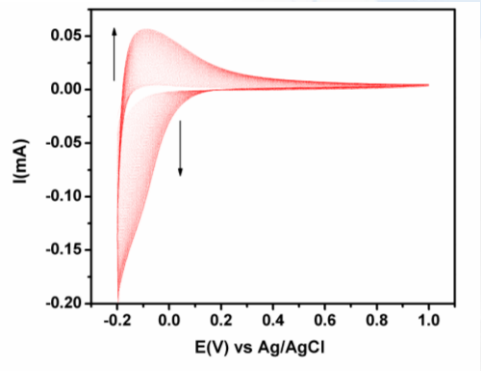


Figure (1): Cyclic voltammogram of nanostructured WO3

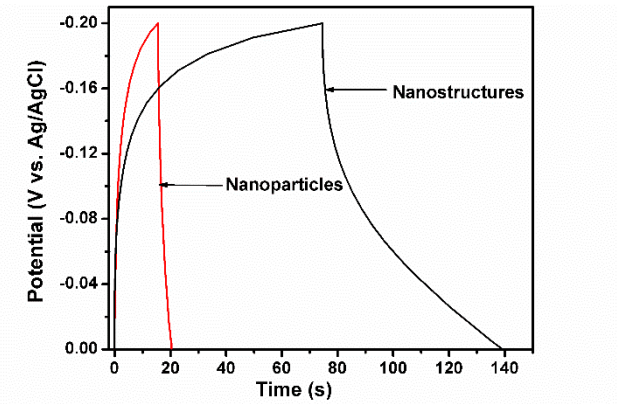


Figure (2): Galvanostatic charge discharge study for WO3 nanoparticles and WO3 nanostructures.

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***Keywords**: Nanostructuring, Tungsten trioxide, Diffusion coefficient, Capacitance.*

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**AMC 03**

# *In situ* growth of silver nanoparticles in poly-vinyl alcohol thin film matrix using green synthesis

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Green synthesis of nanoparticles has gained momentum among the researchers owing due to its eco-friendly approaches (1). Antibacterial, antiviral, antifungal, antioxidant, anti-inflammatory activities of silver nanoparticles and its ability to promote wound healing make it a proper component for wound dressing materials and other applications. This study investigates an effective and biological approach of a novel thin film preparation based on polyvinyl alcohol (PVA) with silver nanoparticles (SNPs) generated within the matrix using plant extract as a bioreducing agent. The successful incorporation of SNPs into the polymer matrix was confirmed by TEM, SEM, and EDX analysis. The characterization studies revealed that the silver nanoparticle was found to be in the range of 10-40 nm. Evaluation of antimicrobial activity on Staphylococcus aureus (ATCC 25923), Escherichia coli, Klebsiella pneumoniae and diploid fungus Candida albicans using disc diffusion and agar cup method confirmed the effective performance of the PVA- SNPs film. The film was biocompatible to L929 and HaCat cell lines (2) and hence could be applicable for wound dressing materials. The method used is simple, greener, rapid, cost effective in producing a biocompatible film with variable applications in health care and food packaging industries.

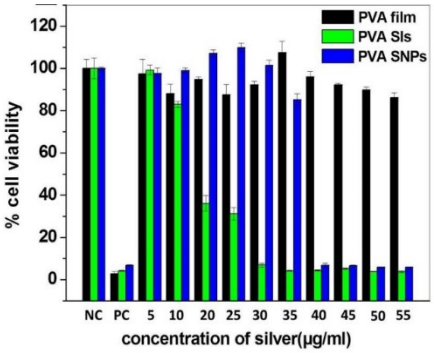


Fig 1: Cell compatibility study on HaCaT cells determined by MTT assay after exposure to SNPs and silver ion (SIs) for 24 hr

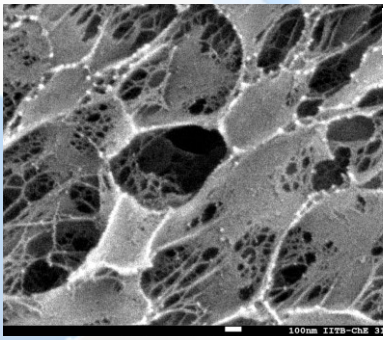

Fig 2: CRYO SEM images of PVA-AgNPs

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***Keywords:*** *Silver nanoparticles, Polyvinyl alcohol, Antibacterial studies, Green synthesis*

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**AMC 04**

# Synthesis and electrochemical characterization of MnFe2O4 nano-ferrites in different electrolytes

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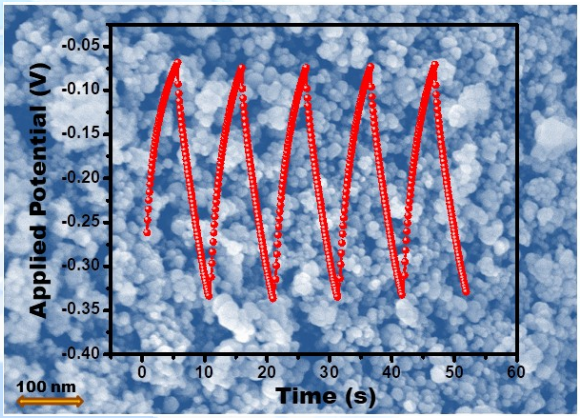
Manganese ferrite nanoparticles have been synthesized successfully by thermal decomposition method using acetylacetonate salts of Mn2+ and Fe3+. XRD confirms the formation of crystalline, pure cubic spinel structure of Mn-ferrite. UV-VIS spectroscopy technique was acquired to calculate the band gap of the nanoparticles from the absorption spectra. FTIR study validates the formation of spinel phase by showing its characteristic peaks at 593 cm-1 and 452 cm-1. FEG-SEM showed that the particles are spherical and the mean particle size ranged ~18.9 nm. The main focus is on the material preparation, structural characterization and the inscribed mechanism that occurred with change in the electrolytes. The present study was executed to investigate the electrochemical behaviour of Mn-ferrite in different electrolytes like NaOH, KOH, H2SO4, PBS buffer, etc. since a material behaves differently to every cation and anion of the electrolyte solution. Electrochemical performance of MnFe2O4 was evaluated using cyclic voltammetry (CV). The voltammograms were obtained using Pt as working electrode in the potential window of 1V at the scan rate of 50mV/s. The cyclic stability of the electrode material is a crucial parameter to rank the performance of the energy storage applications. No single electrolyte can fulfil all the requirements; as from this work, we can conclude that the oxidation potential and the reduction potential vary from one electrolyte to the other, the choice of electrolyte is a primary criteria essential in designing an electrochemical capacitor. Galvanostatic charge/discharge (GCD) was studied upto 1000 cycles in 2M NaOH to understand the stability of the material. Till 7000 s there was no drop in potential after which 20% drop in potential was observed which gives an understanding that the electrode material has good stability in basic media. The results obtained from this study will be useful for further applications such as magnetic materials, semiconductors, sensors and energy storage devices.

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***Keywords**: MnFe2O4, Nanoparticles, Electrolyte, Electrochemical performance.*

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**AMC 05**

# Recyclable functionalized graft biodegradable smart materials for waste water treatment and reuse

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Water contamination and its purification to ensure a healthy life is a global concern. It's indeed a herculean task to prevent organic pollutants and toxic heavy metals from contaminating water, but nonetheless sincere efforts are being made. The present study highlights the application of science and technology being developed to improve the purification process of contaminated water for reduction of impurities to acceptable levels. Water soluble synthetic polymers have been widely explored to extract organic contaminants, while biodegradable polymers are being used for elimination of toxic metals from water(1). A composite of polymers and their advancement as microspheres that are able to extract both these types of contaminants simultaneously by the principle of adsorption has been exemplified in this work. Composite polymers have been made by grafting temperature responsive smart polymers on to the natural polymer pullulan. A series of novel water soluble temperature responsive graft smart materials have been synthesized using ceric ammonium nitrate redox initiator and characterized by FT-IR, DSC, GPC, and NMR. The propensity of these polymers was analysed by UV absorbance method for removal of organic impurities such as pesticides, herbicides and for inorganic heavy metal impurities using ICP-OES. These smart materials have individually shown an elimination of more than 90% for respective contaminants. Moreover, the conversion of these materials by spray drying into microspheres has increased the potency by many folds. These microspheres have also been characterized by SEM for their surface morphology and characteristics. The graft polymers and their microspheres have also been tested for their potential to eliminate contaminants from industrial waste water. A tremendous reduction in Chemical Oxygen Demand (COD) and Biochemical Oxygen Demand (BOD) has been observed by the application of these materials to industrial effluents. The studies reveal applicability of these materials to remove organic and inorganic impurities simultaneously from water by adsorption. Thus, exhibiting efficiency and advantages over conventional water management techniques due to a high reproducibility in synthesis, properties and elimination spectrum.

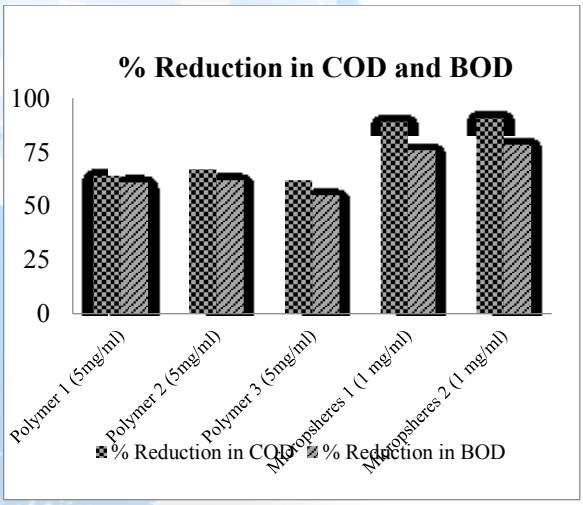


Fig. Reduction in COD and BOD from CETP water

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***Keywords***: *Water management, Smart polymers, Adsorption, Microspheres*

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**AMC 06**

# Exploring biodegradable thermoresponsive material for controlling the environmental pollutants from waste water

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Water is one of the basic necessities required for the sustenance and continuation of life. Pharmaceuticals, dyes, herbicides and pesticides have become chemicals of emerging environmental concern in recent years. Release of this waste water into the environment creates a significant footprint and may also create various other hazards. Hence the availability of fresh water resources has been declining over the years because of the improper management of water (1). To avoid water pollution, it is essential to treat waste water for the removal of pollutants before being discharged into the natural water bodies. One of the ways to achieve this is by use of water soluble polymers that extract organic and metallic contaminants, from waste water. By grafting a natural polymer to a thermo-responsive polymer with a desired lower critical solution temperature (LCST) having the dual ability to adsorb and extract organic, herbicide, pesticide and pharmaceutical impurities from water by the principle of adsorption at LCST. Homopolymer of N-isopropylacrylamide was synthesized via free radical polymerization to give poly(N-isopropylacrylamide) [NIPAM] and it was grafted on surface functionalized biodegradable polymer by DCC coupling mechanism to obtain functionalized chitosan graft NIPAM (fCgN). Structural characterization of fCgN was done by 1H-NMR (Nuclear magnetic resonance spectroscopy) and cloud point confirmation using DSC (Differential Scanning Calorimetry). The fCgN showed prominent adsorption properties for toxic chemicals viz. antibiotics, pesticides and herbicide which are often found in waste water. The fCgN showed maximum adsorption at concentration 5mg/ml for ofloxacin (72.67%), ciprofloxacin (91.81%), chlorpyrifos (49.66%), 2, 4-dichlorophenoxyacetic acid (65.34%). From our studies we can conclude that fCgN biodegradable polymer has an ability to remove significant amount of impurities in ‘one pass’ due to the presence of unique combination of functionalities.

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***Keywords**: Water management, LCST, Smart polymers*

**AMC 07**

# Self-assembled chemisorbed film of tetraaminopalladium(II) phthalocyanine for simultaneous voltammetric determination of ascorbic acid, dopamine and uric acid

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In this study, the palladium(II) tetraaminophthalocyanine (PdTAPc) was synthesized and characterized with different analytical techniques to confirm its purity. The synthesized PdTAPc was immobilized on the electrode surface through self-assembled monolayer (SAM) technique. The immobilized PdTAPc on glassy carbon electrode (GCE) was characterized by XPS, Raman spectroscopy and cyclic voltammetry. The Raman spectra and XPS indicated the modification of the electrode surface with the PdTAPc film (GCE/PdTAPc) by chemisorption. The chemisorbed electrode slightly blocked the charge transfer of K4Fe(CN)6 redox probe. The electroactive species PdTAPc on the electrode surface was used for the sensing of ascorbic acid in the concentration range of 1-25 µmol L-1 and the peak current as well as sensitivity of ascorbic acid species was enhanced by using MWCNTs decorated on the PdTAPc modified GCE (GCE/MWCNTs/PdTAPc). The MWCNTs dispersed PdTAPc modified electrode was used for the simultaneous determination of ascorbic acid (AA) in the concentration range 3-24 µmol L-1, dopamine (DA) 2-16 µmol L-1 and uric acid (UA) 5-40 µmol L-1 respectively and the peaks were clearly separated without any overlapping from one another. The correlation coefficient (r) was found to be 0.9910, 0.9893 and 0.9982 with a limit of detection (LOD) 1.0, 0.60 and 1.50 µmol L-1 (S/N=3) respectively for AA, DA and UA biomolecules. The sensitivity for the simultaneous determination of the biomolecules with MWCNTs modified electrode was high and can be determined without any interference. The sensitivity was found to be1.0149, 1.9303 and 0.4328 mA µmol-1 cm-2 respectively for AA, DA and UA compounds. The modified electrode was also successfully applied to the determination of AA, DA and UA in urine samples.

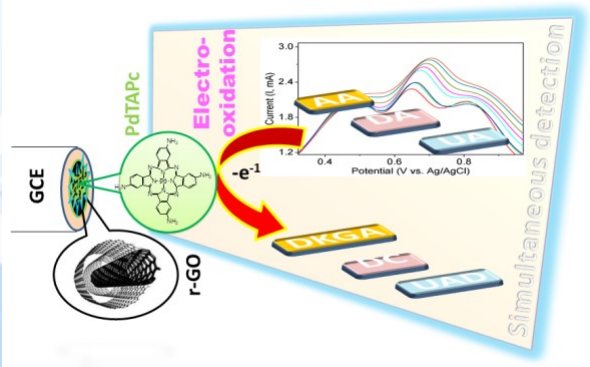


Fig. 1. Schematic representation of chemisorbed PdTAPc-SAM film modified GCE for the simultaneous detection of AA, DA and UA.

***Keywords***: *PdTAPc. XPS. Cyclic Voltammetry. Ascorbic acid. Dopamine. Uric acid. Multiwalled carbon nanotubes.*

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**AMC 08**

# Synthesis of gold nanoparticles and their antioxidant activity

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Recently, there has been growing interest in using surface and plasmonic properties of metal nanoparticles in medical applications because of their properties like easy surface functionalization, and dispersion in water.(1)

Gold nanoparticles (AuNPs) have a remarkable capacity to absorb or scatter a light of broad range of wavelength including visible to infrared depending on size and shape. This property is widely explored in biomedical imaging, cancer therapy, catalysis, sensors and photonic devices.(2)

AuNPs are synthesised by reducing Au(III) ions to Au(0). Various reducing agents suitable for this reduction are reported. Morphological properties like shape and size of AuNPs depend on the strength of reducing agents. And these morphological properties can be observed from UV-Visible spectroscopy and transmission electron microscopy (TEM) analysis.

We synthesised AuNPs by three different methods using three different reducing agents. Viz. chemical reduction by tri-sodium citrate, seed mediated synthesis using pyrogallol as reducing agent and seedless synthesis using ascorbic acid and sodium borohydrate as reducing agent.

The samples were analysed using UV-Visible spectroscopy and TEM to monitor their physiological properties. Shapes of AuNPs were found to be spherical (~11nm), mixture of different shapes (polydisperse, ~15nm) and rods (19.5*6.5 nm) respectively.

All nanoparticle samples were tested for antioxidant assays viz. superoxide radical scavenging assay, DPPH assay and peroxide radical scavenging assay.

% antioxidant activity was calculated using formula:
% antioxidant activity= [(A0-A)/A0]*100 where,
A0= Absorbance of blank
A= Absorbance of sample

Table 1: % antioxidant activity of AuNPs

| S. No. | AuNPs synthesis method | % Antioxidant activity | | |
|---|---|---|---|---|
| | | Superoxide radical scavenging assay | DPPH assay | Peroxide radical scavenging assay |
| 1 | Chemical reduction by tri-sodium citrate | 76.4 | 72.7 | 74.2 |
| 2 | Seed mediated synthesis | 68.9 | 64.8 | 65.3 |
| 3 | Seedless synthesis | 72.0 | 67.4 | 70.5 |

Values of % antioxidant activities obtained from above mentioned formula are listed in table (1).

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***Keywords***: *Nanoparticles, Antioxidant, Morphological properties*

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**AMC 09**

# Assessment of enzymatic activity and cell cytotoxicity of ligand assisted modifications in antioxidant activity ceria nanoparticles

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It is well established that cerium oxide nanoparticles (CeO2NPs) have ability to scavenge free radicals by switching between its two oxidation states Ce3+ (high SOD mimetic activity) and Ce4+ (high catalase mimetic activity). CeO2NPs have limited enzyme mimetic activity in some biological systems due to differences in intracellular pH and limited specificity and selectivity towards different radicals.

CeO2NPs can bind with phosphorous based groups at its surface (1). We hypothesized that functionalizing CeO2NPs with different electron withdrawing (TTMPP) and donating groups (TEP) will increase its stability, activity and solubility in biological system. It is evident from UV-spectrometry, XPS and TEM that the ceria nanoparticles undergo a change in oxidation state after functionalization with phosphorus based ligands depending upon the property of ligands.

Assessment of SOD and catalase mimetic activity of functionalized CeO2NPs using cell free systems indicates the CeO2-x functionalized with TTMPP gives catalase activity while CeO2 functionalized with TEP gives SOD mimetic activity. Reversal of the redox property of functionalized ceria is also confirmed by the PL spectroscopy. In vitro analysis of bare and functionalized CeO2NPs were assessed on the normal (WRL 68) and cancerous (Hep G2) cells lines. Functionalized CeO2NPs is hypothesized to show lower cytotoxicity (oxidation state dependent) and promote antioxidant activity on normal cells. It is also expected to accelerate the cytotoxic effect in cancerous cells by promoting pro-oxidant effect and selectively reduce cytotoxic effect on the normal cells. This study will help researchers to synthesize functionalized nanoparticles with higher selectivity and solubility in biological system.

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***Keywords***: *Ceria nanoparticles, TEP, TTMPP, Anti-oxidant and pro-oxidant activity.*

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**AMC 10**

# Yolk-shell composite cathode for high performance Li-S batteries

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**Introduction:** Electrical energy storage systems with high specific energy and long cycle life, is one of the most crucial needs for mankind in today's world. Elemental sulfur (S), grab special attention as a cathode material owing to their high theoretical capacity (1673 mAh/g) with a theoretical specific energy of 2600 Wh/kg.(1) Moreover, natural abundance of sulfur (~ 3% of earth's mass) makes the cathode material low cost, and it is also environmental friendly. In addition, the low operating voltage (~ 2.1 V) of Li-S batteries can also strengthen the safety of the large format cells. Despite these merits, commmertialization of Li-S battery is hindered by certain flaws.We present here a strategy to fabricate a synergistic composite cathode material which could be tackling the drawbacks. Sulfur (S)-conducting polymer yolk shell structure is fabricated. The yolk-shell structure of sulfur(S)-conducting polymer will provide buffer space for the volumetric expansion of sulfur during lithiation and shell prevents the direct contact of ploysulfides from electrolyte.

**Experiment Section:** In this study we report a surfactant assisted method for the synthesis of sulfur nanoparticles by an acid catalyzed precipitation of sodium thiosulphate in the presence of anionic surfactant. To coat with polymer, the sulfur particles was dispersed in 5mM 100 mL of SDS solution. To prepare the sulfur-polymer yolk-shell structures, the powder of the core-shell particles was sealed into a quartz tube and heated at 140°C for 6 hours in argon atmosphere.

**Result and discussions:** The XRD analysis reveals that all diffraction peaks of the sulfur can be indexed to the crystalline S8 ; which are in good agreement with the JCPDS file no- 08-0247. The samples exhibit single phase orthorhombic structure with average crystallite sizes 76 ± 2 nm. All the characteristic peaks of XRD pattern of core and yolk shell match with sulfur XRD. To estimate the actual sulfur content in the composites, TGA is carried out under oxygen atmosphere. The weight loss is ~ 12 % higher in case of yolk structure as compare to core shell structure, this may act as void to accommodate volume expansion during lithiation. To confirm the presence of polypyrrole, the core and yolk shell samples were also characterized by FTIR. Figure 1 (a)-(b) shows the TEM images of the synthesized sulfur-polypyrrole (S-PPy) yolk shell. It can be seen that the synthesized S-PPy is in the form of ~80 nm spherical particles, which are attached to each other forming continuous connecting network with caterpillar like morphology and it established the formation of PPy layer on S particles.

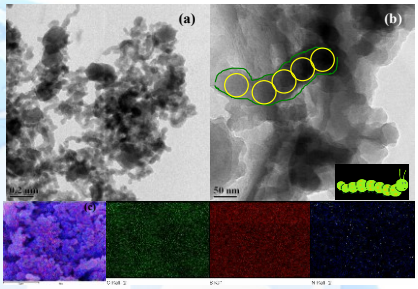


Figure (1): (a)-(b) TEM images of S-PPy yolk shell (c) Elemental mapping of S-PPy yolk shell

In order to confirm the existence and spatial decoration of C and S in nanocomposite, Kα spectral mapping was carried out (Figure 4(c)). In addition to make a buffer space inside the conducting polymer shell, the heat treatment also ensures that all the sulfur particles are well coated and detained by conducting polymer to efficiently trap sulfur from direct contact with electrolytes. The yolk-shell material exhibited a stable capacity of 465 mAh g-1 at 0.2 C after 200 cycles.

**Conclusion:** We fabricated a synergistic composite cathode which could be promising future material. 70-80 nm spherical shape sulfur particles are fabricated by organic acid catalyze thiosulphate disproportionation reaction. TGA analysis confirms the loss of around 12 % of active materials in yolk structure as compare to core and may act as void to accommodate volume. The yolk-shell material exhibited a stable capacity of 465 mAh g-1 at 0.2 C after 200 cycles, representing a promising future for industrial scale Li-S batteries

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***Keywords***: *yolk shell, Li-S battery.*

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**AMC 11**

# One pot green synthesis of Naphth[1,3]oxazine derivatives using Boron Sulphonic Acid as a Heterogeneous Acid Catalyst

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Naphthoxazine derivatives are found to be an integral part of natural products exhibiting various pharmacological properties[1]. Many such compounds are reported as analgesic, anticonvulsant, antibacterial and anticancer agents. The simplest way to synthesize Naphth[1,3]oxazine derivatives is Betti reaction[2]. It is an acid catalysed multicomponent reaction of aldehyde, primary or secondary amine and α-naphthol. The reaction has been reported with various homogeneous as well as heterogeneous catalysts such as Bronsted acid catalysts such as chlorosulphonic acid, $Fe(HSO_4)_3$, $Sr(OTf)_2$ , heteropoly acid catalysts like cation-exchange resins, silica supported perchloric acid , $FeCl_3.SiO_2$, silica sulfuric acid and MCM-41-N-propylsulfamic acid. But, many of these catalysts suffer through the limitations of high cost, poor reusability, complexity in methods of preparation and poor acid strength.

In present work, we have studied the use of boron sulphonic acid (BSA) as a heterogeneous catalyst[3] for Naphth[1,3]oxazine. BSA was synthesised and characterised by FT-IR and TGA. The reaction conditions were optimised for synthesis of Naphth[1,3]oxazine. Good to excellent yields were observed for Naphth[1,3]oxazine derivatives.

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***Keywords:*** solid acid catalyst, boron sulphonic acid

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**AS 01**

# Photophysical aspects of perylene diimide derivatives in preorganized and self-assembled systems in aqueous medium

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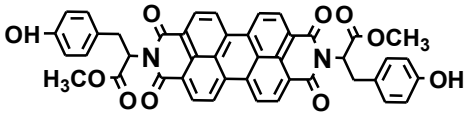
Perylenebisimides (PDI) dyes are among the most widely studied functional dyes and have numerous potential applications owing to their outstanding characters such as strong absorption in the visible region, highly electron deficient nature and great thermal stability. PDI dyes have been applied as pigments, fluorescence sensors and n-type semiconductors in organic electronics and photovoltaics [1]. However, the studies on the various phothophysical aspects of perylene bisimide dyes have been restricted mostly to organic media due to the exceptional hydrophobic nature of these dyes.

In this presentation, we would like to report the results of our comprehensive study on the photophysical as well as supramolecular aspects of a newly synthesized water soluble L-tyrosine and its methyl ester derived perylenetetracarboxylic diimide (PDI) derivative in aqueous medium. PDI derivatives are strongly hydrophobic hence they form aggregates in aqueous medium which leads to emission quenching. Effective deaggregation of L-tyrosinyl-PDI was achieved through the complexation with preorganized host such as β-cyclodextrin in aqueous medium. Job's plot experiment clearly shows 1:2 (PDI:β-CD) complex formation of PDI with β-CD at pH 7.5. In a similar note, self-assembled systems typically anionic micelles also lead to the spontaneous deaggregation of the PDI derivative at relatively lower CMC in aqueous medium.




L-tyrosine (methyl ester) perylenediimide


L-tyrosine perylenediimide

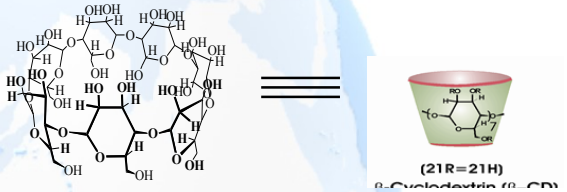



Chart1: Chemical structures of neutral and anionic forms of L-tyrosine and methyl ester derivatised perylenediimide and β-Cyclodextrin

To study the interaction of the PDI derivative with self-assembled supramolecular systems by steady state absorption, fluorescence, time resolved spectroscopic techniques will also be presented.

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**AS 02**

# Modulation of prototropic tautomerism in chrysazine through host-guest interactions

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Present study explores the interesting effect of two p-sulfonatocalix[n]arene hosts (SCXn, n = 4 and 6) on the excited-state prototropic tautomerism of a model antitumour drug, Chrysazine (CZ). The CZ molecule in its electronic ground state exists in the normal form (N), which upon electronic excitation undergoes prototropic tautomerization, converting its N* form to the tautomeric form (T*).[1] In the presence of the SCXn hosts, CZ shows significant quenching of its fluorescence intensity along with a substantial change in the spectral shape. Thus, at the highest host concentration, the emission band corresponding to T* form, which is initially much stronger than the emission band of N* form, almost becomes at par with respect to the relative intensity, clearly indicating largely diminished tautomerization of CZ upon its interaction with the two host molecules. Interestingly, the extent of decrease in the tautomerization process is found to be larger in the case of SCX6-CZ system as compared to SCX4-CZ system, although the binding interaction is found to be weaker in the former case than the latter.

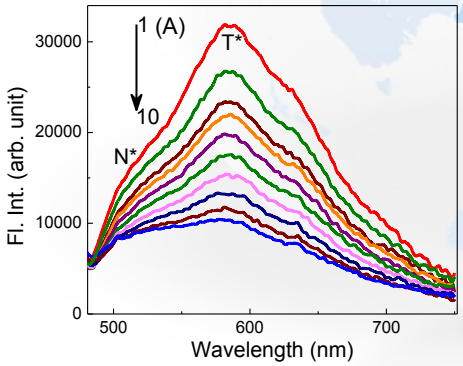


Figure (1): Emission spectra of CZ (3 μM) in water with 0, 2.0, 3.4, 4.4, 6.7, 9.4, 12.5, 17.2, 23.3 and 31.0 mM SCX4 (1-10).

The decrease in the tautomerization of CZ in the presence of the two hosts is justifiably correlated with the formation of new intermolecular H-bonds between CZ and the sulfonate groups at the portals of the SCXn hosts which rupture the pre-existing intramolecular H-bonds within the CZ molecule and thus modulates the tautomerization process.[2] It is proposed that the new intermolecular H-bonds between CZ and the sulfonate groups are formed more favourably in the CZ-SCX6 system than in the CZ-SCX4 system, due to the more appropriate orientation of the dye with respect to the host cavity in the former system as compared to the latter system. This proposition is well supported by the detailed quantum chemical calculations whereby it is indicated that while CZ is partly encapsulated into the macrocyclic host cavity of SCX4, the dye remains just externally bound to the portals of the SCX6 host as exo-complexes, favouring intermolecular H-bondings. Results from the present study emphasize that not only the localized binding pockets provided by the biological hosts, but also the orientations and specific interactions of the dye/drug with the host are important parameters in determining the course of any tautomeric process occurring in natural systems.

| | Binding constant obtained using equation $\Delta I_N = \Delta I_N^{\infty} \frac{K_{eq}[H]_0}{1+K_{eq}[H]_0}$ | Binding constant obtained using equation $\Delta I_T = \Delta I_T^{\infty} \frac{K_{eq}[H]_0}{1+K_{eq}[H]_0}$ | $K_T$ α $I_T/I_N$ | |
|---|---|---|---|---|
| | | | $I_{T0}/I_{N0}$ (free dye) | $I_{T\infty}/I_{N\infty}$ (bound dye) |
| SCX4 -CZ | $K_{eq}$ = 135 $M^{-1}$ | $K_{eq}$ = 118 $M^{-1}$ | 2.1 | 0.6 |
| SCX6 -CZ | $K_{eq}$ = 79 $M^{-1}$ | $K_{eq}$ = 81 $M^{-1}$ | 2.1 | 0.3 |

Table 1: Binding parameters and tautomerization constants for CZ-SCXn system.

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***Keywords:*** *Tuatomerization, Prototropic, Intramolecular, Inhibition.*

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**AS 03**

# Antidiabetic activity of a compound isolated from *L. racemosa* leaves in STZ induced diabetic Wistar rats

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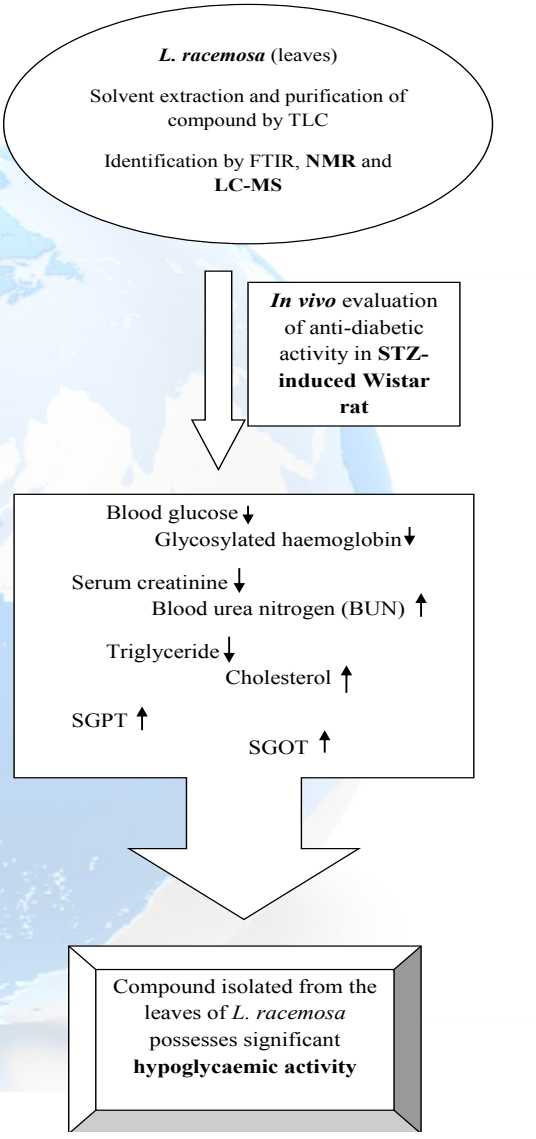
Mangroves are salt tolerant plants grow along the coastline. India has about 70 mangroves species, among them about 24 growing luxuriantly along Mumbai coast. The mangrove plants proved to have various medicinal properties such as antidiabetic, antibacterial, antioxidant, anti larvicidal etc. The current study was framed to evaluate the hypoglycaemic activity of the compound isolated from L. racemosa mangrove plant. The main purpose was to find out new antidiabetic compound(s) from mangrove plant. The plant was collected from Ratnagiri coast, Mumbai in the month of May.

**Methods:** Solvent extractions followed by column and thin layer chromatographic techniques were used to purify the compounds. 1H-NMR and 13C NMR spectroscopy and also LC-MS was used to identify the purified compounds which might have antidiabetic property. In vivo antidiabetic activity was evaluated in a streptozotocin-induced Wistar rat. Blood glucose, glycosylated haemoglobin, serum creatinine, blood urea nitrogen (BUN), triglyceride, cholesterol, SGPT, SGOT were determined. Liver, kidney and pancreas histopathology were assessed.

**Results:** Isolated compound showed significant hypoglycaemic activity by reducing elevated glucose level. The histopathology results for the rats that received the compound (500 mg/kg) showed healing feature compared to disease control.

**Conclusion:** Compound isolated from the leaves of L. racemosa possesses significant hypoglycaemic activity.




***Keywords:*** *Mangrove, Antidiabetic, 1H-NMR, Streptozotocin.*

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AS 04

# Evaluation of certain chemical parameters of industrial effluents by spectroscopy

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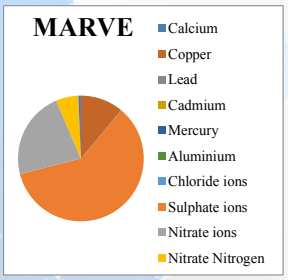
**Background:** Purified water is an integral constituent for the subsistence of healthy life of human beings, plants & animals. Mahim Creek is a creek in Mumbai, India into which the Mithi River drains. Marve Creek is a creek in north-west Mumbai. Located west of Malad, the Oshiwara River drains into it.The instrumental spectroscopic techniques are superior over conventional volumetric and gravimetric estimation with respect to accuracy, sensitivity and reproducibility

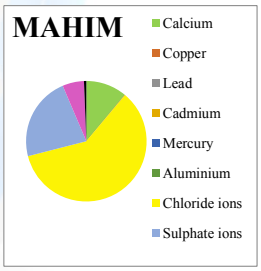
**Methodology:** The present study is limited to the evaluation of certain Chemical species on the basis of spectroscopic techniques. Calcium was estimated by AAS.Ca was treated with HCl forming $CaCl_2$ and the estimation was carried out at 4227A with air pressure of 28psi in a reducing flame. Acetylene was used as fuel.Copper was estimated by AAS.Cu was treated with $HNO_3$ forming $Cu(NO_3)_2$ and the estimation was carried out at 3247A with air pressure of 28 – 30 psi in a oxidising flame. Lead was estimated spectrophotometrically. Pb reacts with dibromohydroxyphenyl porphyrin,1:2 yellow complex and absorbance was measured at 479 nm.

Cadmium was estimated spectrophotometrically .Cd forms a complex with 5,7-dibromo 8 hydroxoquinoline and absorbance was measured at 396 nm.Mercury was estimated spectrophotometrically .Hg reacts with 2-(2-benzothiazolylaza)-p-cresol and absorbance was measured at 650 nm.Aluminium was quantified by Fluorescence spectroscopy by the formation a complex with N-((2-hydroxynaphthalene-1-yl)methylene)acetyl hydrazide (HNMA).The fluorescence of the complex is 450 nm and excitation at 385 nmThe absorbance was determined at 480 nm.Sulphate ions were determined by the formation of $Na_2SO_4$ and the absorbance measurement was carried out at 420 nm.Nitrate ions were evaluated spectrophotometrically by the formation a complex with 2,6-bis(4-methoxy phenyl)-4-phenyl pyrilium perchlorate(PPP).The complex was extracted with Naphthalene and dissolved in DMF and absorbance measurement was carried out at 328 nm.Nitrate nitrogen was estimated by Brucine ($C_{23}H_{26}N2O_4$) method which involves the formation of yellow coloured complex with $H_2SO_4$

**Results:** The results obtained for the water samples from the Mahim creek and Marve creek are tabulated as below:

| Species | Units | Values Mahim | Values Marve | Permissible limits |
|---|---|---|---|---|
| Calcium | Ppm | 235 | 210 | 200 |
| Copper | Ppm | 1.9 | 1.6 | 1.5 |
| Lead | Ppm | 0.09 | 0.07 | 0.05 |
| Cadmium | Ppm | 0.02 | 0.015 | 0.01 |
| Mercury | Ppm | 0.0014 | traces | 0.001 |
| Aluminium | Ppm | 0.34 | 0.25 | 0.2 |
| Chloride ions | Ppm | 1200 | 1140 | 1000 |
| Sulphate ions | Ppm | 455 | 430 | 400 |
| Nitrate ions | Pppm | 125 | 110 | 100 |
| Nitrate Nitrogen | Ppm | 14 | 12 | 10 |




**Conclusion:** As per the results obtained it seems that water sample of Mahim creek is more polluted than Marve creek.Many procedures as directed by the Enviromental Protection Agancy (EPA) and Maharashtra Pollution Control Board (MPCB) must be strictly adhered.

**References:**
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2. and heavy metals in water samples from Itaogbolu area of Ondo-State, Nigeria, African
3. Journal of Environmental Science and Technology, 4(3), pp 145-148. 2. Adeyeye EI, (1994),
4. ASTM International, (2003), Annual Book of ASTM Standards,World Health Organization (W.H.O.) (1998) Guideline for drinking waterquality

***Keywords:*** industrialization, AAS, spectrophotometric, fluorescence spectroscopy, EPA

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**AS 05**

# Compatibility studies of anti-rheumatic drugs for dual drug delivery

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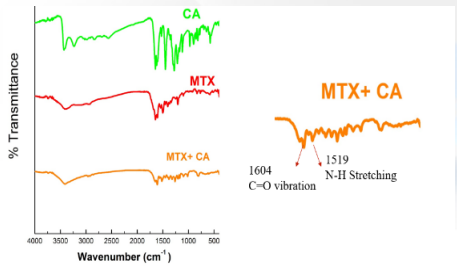
**Objective:** To assess compatibility of anti-rheumatic drugs for developing a novel formulation for combination therapy. The potential physical and chemical interactions can affect the chemical nature, stability, and bioavailability of drugs and subsequently their therapeutic efficacy and safety. Thus, it is an important aspect prior to formulating a carrier system for drug delivery.
**Method:** Analytical techniques such as FTIR, DSC and HPLC were used to assess possible interaction between methotrexate (MTX) and an anti-oxidant [Quercetin (QE) or Caffeic acid (CA)]. Stability of the drug in mixture (1:1 ratio, w/w) stored at 40±2°C and 75±5% RH for 1 and 3 months was also assessed.
**Results:** The FTIR and HPLC data showed no evidence of interaction in either combinations (MTX-CA and MTX-QE). While DSC data indicates possibile interaction between MTX and QE. Similar results were observed when the drug combinations were analysed after storage under the specified conditions.
**Conclusion:** The results showed no physico-chemical interactions in MTX-CA combination and thus may be suitable for further studies for developing dual drug formulation. XRD studies are being carried out presently to confirm the results obtained for both the combinations.

a)




b)

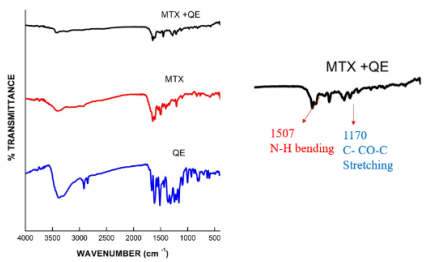
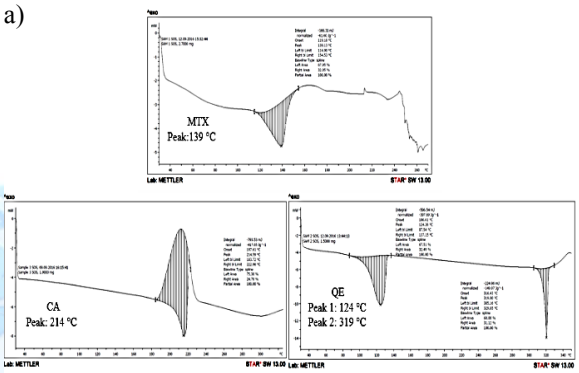



Figure (1): FTIR Spectra of a) MTX-CA; b) MTX-QE

a)




b)

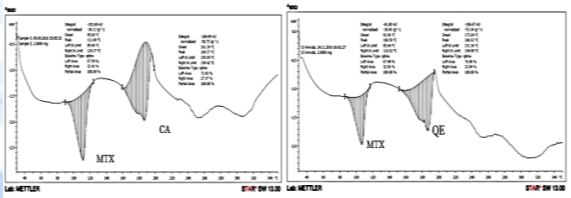



Figure (2): DSC Graph of a) MTX, QE and CA; b) MTX-CA and MTX-QE

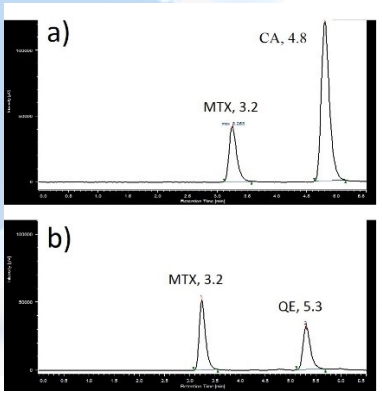



Figure (3): HPLC Chromatogram of a) MTX-CA; and b) MTX-QE

**References:**
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***Keywords**: methorexate, caffeic acid, quercetin compatibility, DSC, FTIR, HPLC*

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**BTE 01**

# Induced pluripotent stem cell derived cardiomyocytes - a platform for cardiac tissue engineering

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Cardiovascular diseases (CVDs) such as Myocardial Infarction, Myocardial Ischemia, Atherosclerosis, Arrhythmia and Cardiomyopathies are major cause of morbidity worldwide. The World Health Organization estimated that annually 17.5 million populations per year of all global death are due to CVDs. Most CVDs are associated with loss of functional cardiomyocytes (CMs) that have limited self-renewal or regenerative potential at adult age and hence insufficient to compensate the lost CMs. Recently, significant advancements are made in the field of induced pluripotent stem cells (iPSCs) aimed to find new therapeutic approaches for the treatment of CVDs. The iPSCs as an alternative to pluripotent embryonic stem cells (ESCs) are derived by direct reprogramming of somatic cells using reprogramming factors such as Oct4, Sox2, Nanog and Lin28 (OSNL) or Oct4, Sox2, Klf4 and c-Myc (KOSM). Fully reprogrammed iPSCs resemble ESCs in their morphology, gene expression and phenotype to self-renew and differentiate into all three germ layers including CMs. Cardiac differentiation can be induced in human iPSCs by various methods such as co-culture with embryoid bodies (EBs), treating them with protein factors and GSK pathways etc. However, CMs derived from human ESCs and iPSCs do not differ significantly with respect to sarcomeric organization, cardiac gene expression, responsiveness, and beat rate variability. Consequently, a number of studies have used iPSCs as an alternative to ESCs for generation of CMs whereas produced the cell type with low efficiency. Use of iPSCs offers an advantage of being patient-specific autologous cell source which in turn is expected to minimize the chances of immune rejection. Furthermore, when isolated from patient's own adult somatic cell, it avoids ethical, legal and social issues associated with ESCs. However, precise mechanism behind reprogramming and functionality of reprogrammed cell is still elusive. In this study we will summarize the recent methods for cardiomyocytes differentiation with improved efficiency and scalability including cardiac tissue engineering and regenerative medicines.

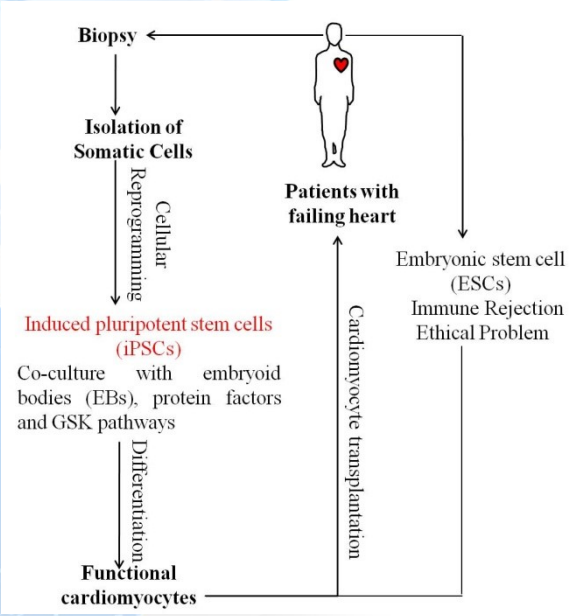


Figure (1): Generation of functional beating cardiomyocytes from induced pluripotent stem cells.

***Keywords***: *beating cells, cardiac diseases, differentiation, stem cells, tissue engineering*

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**BTE 02**

# Effect of growth hormone–releasing hormone and IGF-1 on human placenta derived mesenchymal stem cells proliferation and differentiation

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Increasing evidence highlights the multipotent potential of mesenchymal stromal cells (MSCs), produced in peripheral tissues, bone marrow etc. to promote tissue regeneration and hence cell-based therapies. In this regard, the human placenta has attracted attention for translational research due to its immunomodulatory properties, large stem cell number in tissue, and ease of availability for clinical experimentation.

The placenta plays the role of an endocrine organ in providing the foetus nutrition and also exerts some control over maternal hormones during gestation through expression of several hormones including the growth hormone releasing hormone (GHRH), placental growth hormone (GH) and insulin like growth factor (IGF-1). While on one hand, the role of GHRH in the placenta is unclear and there are only speculations of a paracrine role for GHRH in the placenta; on the other hand, GHRH and its analogues have been used to pre-condition bone marrow MSCs for cell based therapies in treatment of angiogenesis and GHRH antagonists are being considered for cancer therapy, due to its role in regulating somatic growth.

Given this scenario, we studied the effect of GHRH and IGF-1 on the proliferation and differentiation of human placenta derived MSCs. GHRH and IGF-1 by themselves and in combination stimulated faster proliferation of MSCs compared to controls. The combination of GHRH and IGF-1 also enhanced the rate of osetocytic and chondrocytic differentiation. GHRH was particularly effective in inducing chondrogenesis in p-MSCs. Our study opens the possibility for hitherto unidentified roles for GHRH in the placenta.

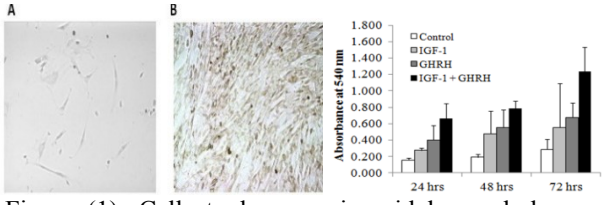


Figure (1): Cells took on a sigmoidal morphology after isolation and adherence to plastic (Figure A). After 7 days of culture, flasks were confluent (Figure A & B). Graph showed GHRH and IGF-1 increase proliferation of p-MSCs.

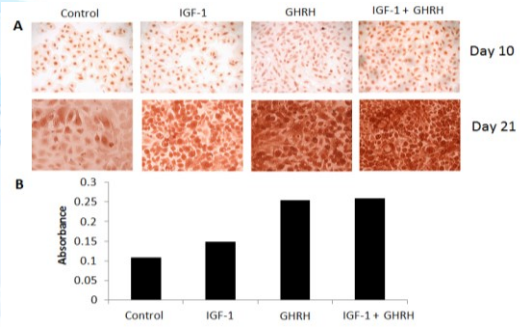


Figure (2): IGF-1 and GHRH increase chondrocytic differentiation of placental MSCs. Cells were stained with Safrain O. B. Shows quantitation of differentiation by measuring safranin O staining on day 10.

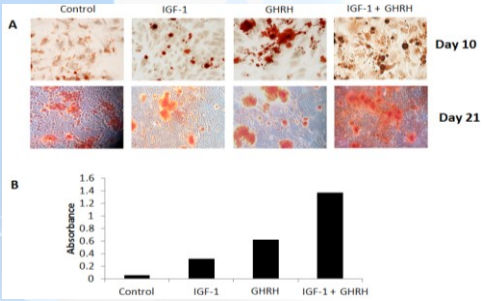


Figure (3): IGF-1 and GHRH increase osteocytic differentiation of placental MSCs. Cells were stained with Alizarin red B. Shows quantitation of differentiation by measuring Alizarin red staining on day 10.

**References:**
[1] Sundell IB, Koka PS. Placental membrane as a source of mesenchymal stem cells. *J Stem Cells* 2011. 5(2): 83-88.
[2] Plotsky PM, Vale W. Patterns of growth hormone-releasing factor and somatostatin secretion into the hypophysial-portal circulation of the rat. Science. 1985. 230 (4724): 461–3.

***Keywords**: placental mesenchymal stem cells, GHRH, IGF-1, differentiation, signalling.*

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**BTE-03**

# Substrate stiffness regulates YAP/TAZ activity in human pluripotent stem cells

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Pluripotent stem cells (PSCs) have the potential to differentiate into any cell type but to differentiate them into specific lineage continues to be a challenge for researchers. While signalling molecules have been well-established to initiate lineage specific differentiation, recently it was shown that biophysical cues from extracellular matrix initiate a cascade of reactions which leads to specific cell fate of PSCs. Substrate stiffness alone has been shown to regulate differentiation of mesenchymal stem cells, with stiffer substrate leading to osteogenic differentiation while lesser stiff substrate leading to adipogenic differentiation. Transcriptional co-activators, Yes-associated protein (YAP) and transcriptional co-activator of PTZ binding motif (TAZ) acts as an intermediating molecule for signalling pathways such as Hippo, TGF-β/BMP and WNT thus playing an important role in tumour suppression and cell proliferation. Recently, YAP/TAZ have been shown to respond to biophysical signals generated extra- and inter-cellularly in mesenchymal stem cells and epithelial cells when cultured on confined substrates or substrates of various stiffness. Stiffer substrate have been shown to upregulate YAP/TAZ levels thus maintaining undifferentiated state of hPSCs, while soft substrate has been shown to differentiate hPSCs into neuronal lineage. However, wheather the substarte stiffness plays a vital role in hPSCs differentiation into endoderm is still remains unclear.

Our aim was to study the expression levels of YAP and TAZ in hPSCs cultured on substrate of varying stiffness. In the present study, we cultured human pluripotent stem cells (hPSCs) on vitronectin coated polyacrylamide gel substrates of various stiffness. Substrates were synthesized using varying concentrations of acrylamide-bisacrylamide solution and stiffness (expresses as Young's modulus in kilopascals, kPa), was assessed using atomic force microscopy. Young's modulus for 10%, 15% and 20% PA gel solutions was calculated to be 1.89kPa, 2.76kPa and 5.34kPa respectively. hPSCs colonies were observed in 20% PA gel substrate and not on 10% or 15% substrate. Expression levels of *YAP* and *TAZ* was studied using real time PCR and western blot. *YAP* expression was downregulated in hPSCs cultured on 20% PA substrate compared to hPSCs cultured on vitronectin coated plastic culture dishes. hPSCs cultured on 20% PA substrate coated with vitronectin showed no expression for endoderm, neuroectodermal and mesoderm specific markers such as SOX17,*PAX6,* and *BRACHYURY*. However, hPSCs expressed *OCT4* indicating that stem cells remain pluripotent even on soft substrate. By modulating stiffness of polyacrylamide gel substrate, we showed that hPSCs remained undifferentiated on soft substrate (~5kPa) which is way less than standard culturing plastic dishes (~1GPa). Our findings imply that soft substrate does not lead to differentiation of hPSCs.

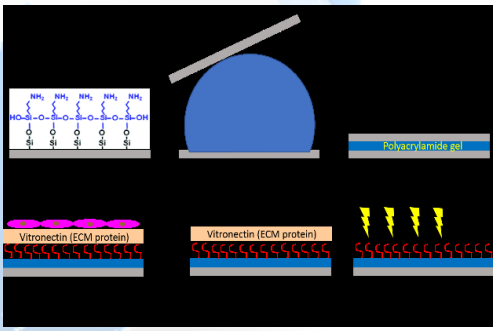


Figure (1): Diagrammatic representation of Polyacrylamide gel (PA) substrate synthesis and hPSCs seeding on the PA substrate.

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1. Engler, A.J., Sen, S., Sweeney, H.L. and Discher, D.E., 2006. Matrix elasticity +directs stem cell lineage specification. *Cell*, *126*(4), pp.677-689.
2. Dupont, S., Morsut, L., Aragona, M., Enzo, E., Giulitti, S., Cordenonsi, M., Zanconato, F., Le Digabel, J., Forcato, M., Bicciato, S. and Elvassore, N., 2011. Role of YAP/TAZ in mechanotransduction. *Nature*, *474*(7350), pp.179-185.
3. Halder, G., Dupont, S. and Piccolo, S., 2012. Transduction of mechanical and cytoskeletal cues by YAP and TAZ. *Nature Reviews. Molecular Cell Biology*, *13*(9), p.591.

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**BCI 01**

# Computational analysis of putative phytase enzymes

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**Background:** Enzymes are biological catalyst and have wide applications in various industries like food, agriculture, chemicals, pharmaceuticals, cosmetics, environment and research. Constant exploration of new enzymes or improvement of current set of enzymes is required to meet the demand of enzyme industry. Evolution of extant enzymes to catalyse novel chemical reactions is a challenging and continual process. Both computational and experimental characterization of novel enzymes belonging to different superfamilies like Oxidoreductases, Hydrolases, Ligases have increased the existing enzyme databases. Computational analysis and predictions of novel putative enzymes can help in assessing the biochemical properties and their evolutionary relationship (1) (2).

**Objective:** The objective of present study is to computationally analyse phytase enzyme candidates to predict their biochemical and evolutionary properties.

**Materials and Methods:** Enzyme databases were searched for non-redundant candidates belonging to a class of phytase enzyme superfamily. The multiple sequence alignment was performed on selected candidates, which was followed by phylogenetic analysis and data interpretation (3) (4).

**Significance:** Phylogenetic clustering and study of biochemical properties of novel or putative enzymes can help in understanding functional diversity, identification of motifs and their selection for enzyme engineering to improve its properties.

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1. Newton MS, Arcus VL, Gerth ML, Patrick WM. Enzyme evolution: innovation is easy, optimization is complicated. Curr Opin Struct Biol. 2018;48:110–6.
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3. Kumar V, Singh G, Verma AK, Agrawal S. In silico characterization of histidine acid phytase sequences. Enzyme Res. 2012;
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***Keywords***: *putative enzyme, phylogenetic clustering, biochemical properties, functional diversity.*

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**BCI 02**

# Using *in silico* methods to design the blueprint for BCL-2 inhibitors

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Members of the BCL-2 family of proteins regulate the process of apoptosis by its promotion or inhibition. Overexpression of the pro-survival anti-apoptotic proteins (Bcl-2, Bcl-xL, Mcl-1) are responsible for tumor maintenance, growth and progression. Although the role of Bcl-2 in apoptosis was widely known and studied computationally, an *in silico* exploration of Mcl-1 and how it differs structurally from Bcl-2 and Bcl-xL had not been clearly elucidated. In order to understand the same, we carried out docking and molecular dynamic simulations on ABT-263 (Navitoclax), an orally active inhibitor of Bcl-2, Bcl-xL and Bcl-w proteins; Obatoclax, a pan-Bcl-2 inhibitor as well as Maritoclax, an Mcl-1 specific inhibitor. Docking studies revealed that binding to the hydrophobic grooves is a prerequisite for action on all proteins of the BCL family and the binding mechanism and chemical space utilization dictates stability as well as specificity of the inhibitor. Molecular dynamic simulations showed that on binding, the α-helices of these proteins exhibited less fluctuations than loop regions, also hydrophobic contacts and hydrogen bonding were observed to be the predominant interactions in the drug-receptor complexes.

Based on the structure of the hydrophobic grooves of Bcl-2 and Mcl-1, we designed some structurally diverse molecules which showed good activity in cell lines preferentially expressing these antiapoptotic proteins. It was observed that there was a satisfactory correlation between the docking scores and actual biological activity, which reaffirms that optimization of binding of molecules to the BCL proteins dictates interaction stability as well as activity.

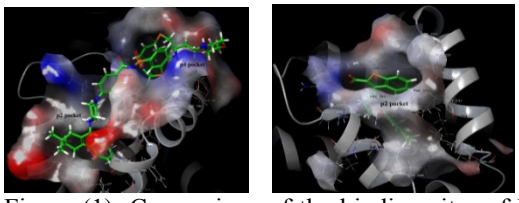

Figure (1): Comparison of the binding sites of Bcl-2 and Mcl-1

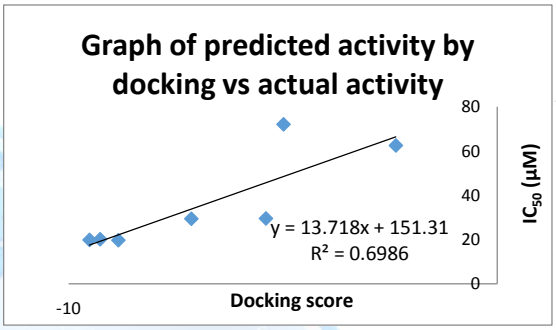


Figure (2): Correlation between docking scores and obtained bioactivity for known as well as designed molecules

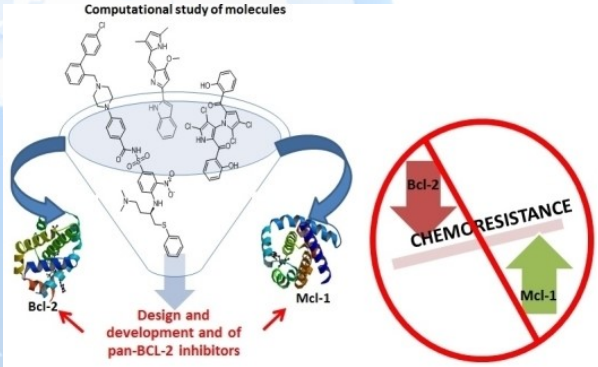


Figure (3): Computational study of the BCL family of proteins may help design molecules to overcome chemoresistance

**References:**
1. Acoca S, Cui Q, Shore GC, Purisima EO. Molecular dynamics study of small molecule inhibitors of the Bcl- 2 family. Proteins: Structure, Function, and Bioinformatics. 2011 Sep 1; 79 (9):2624-36.
2. Dalafave DS, Prisco G. Inhibition of antiapoptotic Bcl-xL, Bcl-2, and Mcl-1 proteins by small molecule mimetics. Cancer informatics. 2010 Jan; 9: CIN-S5065.

***Keywords***: *apoptosis, Bcl-2 inhibitors, molecular docking, molecular dynamics*

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**BCI 03**

# Benchmarking different parameters for computing host-guest binding

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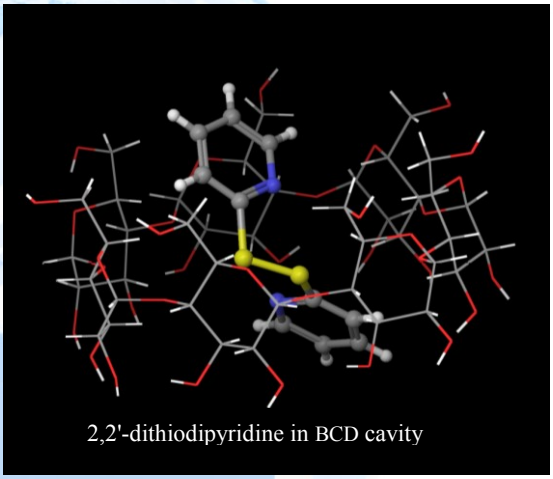
**Background:** Inclusion techniques containing β-cyclodextrin (BCD) are used in drug delivery to enhance the solubility, bioavailability[1] and stability of drugs. The different interactions of complex include non-covalent interactions like hydrogen bonding, ionic bonding, van der Waals forces, electrostatic and hydrophobic bonding[2]. The binding energy of these complexes is calculated using molecular mechanics with Poisson-Boltzmann surface area (PBSA) or the generalized Born Surface area (GBSA) models.

**Methods:** The crystal structures of the complexes were taken from Cambridge Crystallographic Data Centre (CCDC). Optimization of the ligands was done using Gaussian 09. Complexes were formed using Glide v5.8 of Schrödinger suite. Molecular dynamics(MD) studies and binding energy calculations were done using Amber16.

**Results:** The binding energy (BE) of number of molecules were calculated. However, the BE for some illustrative molecules are reported in the table.

| Sr. | Name | Expt ΔG kcal/mol | Calc ΔG kcal/mol | Parameters | | |
|---|---|---|---|---|---|---|
| | | | | PB/GB | mbondi | ε |
| 1 | 1-(2-pyridyl)-2-(4-pyridyl) ethylene | -3.77 | -3.80 | PB | 2 | 2 |
| 2 | 2,2'-dithiodipyridine | -3.29 | -3.08 | GB2 | 3 | 1 |
| 3 | 4,4'-bipyridine | -3.01 | -2.98 | GB2 | 2 | 2 |
| 4 | Naphthyloxy acetic acid | -3.49 | -4.20 | GB5 | 2 | 1 |
| 5 | Nicotinic acid | -1.10 | -1.99 | GB1 | 2 | 1 |
| 6 | (+) Catechin | -5.38 | -5.65 | GB2 | 3 | 2 |
| 7 | (-) Epicatechin | -4.35 | -4.62 | GB8 | 2 | 1 |
| 8 | Epicatechingallate | -3.87 | -4.02 | GB2 | 2 | 1 |

**Conclusion:**
Binding energy for these complexes using different parameters will help to set a standardized protocol with the best parameters.


2,2'-dithiodipyridine in BCD cavity

**References:**
1. Arima H, Yunomae K, Miyake K, Irie T, Hirayama F, Uekama K. Comparative studies of the enhancing effects of cyclodextrins on the solubility and oral bioavailability of tacrolimus in rats. Journal of pharmaceutical sciences. 2001;90(6):690-701.
2. Lodish H, Berk A, Darnell JE, Kaiser CA, Krieger M, Scott MP, et al. Molecular cell biology: Macmillan; 2008.

***Keywords:*** *host-guest complexes, binding energy, MM-PBSA, MM-GBSA*

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**BCI 04**

# Bioinformatic analysis on differential miRNA expression during wheat fungal diseases

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Computational prediction and identification of miRNAs, a class of non-coding RNA their corresponding targets and the channels they are acting through during plant-pathogen interactions have immense applications in breeding disease resistant plant varieties.

Here, we have used ESTs of resistant and susceptible wheat varieties corresponding to Powdery mildew, Leaf rust and wheat Blast diseases for comparing differential expression of miRNAs and their targets. Previously known miRNAs were used for BLAST search against wheat ESTs followed by secondary structure prediction resulted in the identification of putative miRNAs [1]. Number of miRNAs predicted in each resistant and susceptible varieties of wheat after fungal infection differs from 4 to 14 and are predicted to regulate multiple genes either via mRNA cleavage/by translational inhibition. We could find significant overlap in the miRNA expression among the wheat resistant varieties of powdery mildew and blast disease. Predicted miRNAs in resistant varieties of the diseases mostly target glutathione transferase, calmodulin, transcription factor ILR3 etc. which are directly linked with plant defense responses. Similarly, miRNAs from the susceptible varieties target the transcripts of sugar transport protein 13, brown planthopper-induced resistance protein 1, MAPK kinase substrate proteins etc. The induction of specific miRNAs in the susceptible varieties inturn helps the pathogen to grow inside the host.The data obtained show that even though some miRNAs were induced in different varieties, they have specific targets in each conditions.

Table (1): Putative miRNAs obtained in Powdery mildew resistant variety

| miRNAs | Homolog miRNAS | Mature Sequence |
|---|---|---|
| miR1130a | tae-miR1130a | CCTCCGTTCCATAATGTAAGACG |
| miR1436 | osa-miR1436 | ACATTATGGAACGGAGGGAGT |
| miR1136 | tae-miR1136 | TCGTCACAGAAATGGATGTATCTA |
| miR1128 | ssp-miR1128 | CACTTATTTTGGAACGGAGGGA |
| miR1135 | bdi-miR1135 | CCACGACAAGTAATTCCGAACGGA |
| miR1127a | tae-miR1127a | TCCCTCCGTTCGGAATTAC |
| miR1120 | hvu-miR1120 | ACACTCTTATATTATGGGACAGAGGG |
| miR1130b-3p | tae-miR1130b-3p | TCTTATATTATGGGACAGAGGGA |
| miR1120a | tae-miR1120a | ACACTCTTATATTATGGGACAGAGG |
| miR5049e | hvu-miR5049e | ATATTTAGGTTGGAGGGAG |

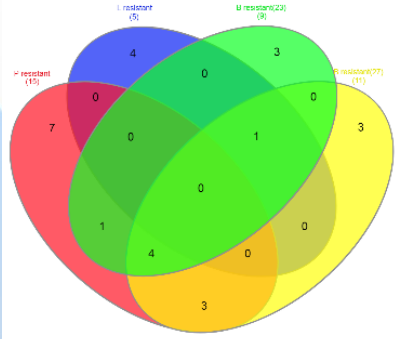


Figure (1): miRNAs in common among disease resistant varieties

**References:**
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***Keywords****: miRNA mining, target prediction, plant defense responses, wheat-fungal diseases*

**BCI 05**

# *In silico* development of efficient L-asparaginase enzyme for acute lymphoblastic leukaemia therapy

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L-asparaginase has been accepted clinically as an anti-tumour agent for the effective treatment of acute lymphoblastic leukaemia and lymphosarcoma. This enzyme also possesses L-glutaminase activity and causes immunological problems. Hence, efforts have been made to develop mutants with lower or no glutaminase activity. In the present study, a homology model of L-asparaginase obtained from *Pectobacterium carotovorum* was docked and compared with its mutants for activities, analysed for molecular dynamics and structural stability. A total of 5 *in silico* mutants were developed using single point mutation and evaluated for ligand binding for both L-asparagine and L-glutamine. The mutants, Y306L, showed -5.89 and -5.04 while the wild L-asparaginase revealed -5.50 and -5.12 binding energies for L-asparagine and L-glutamine, respectively. Molecular dynamics analysis denoted that mutant protein is more stable in RMSD, RMSF and radius of gyration to that of wild-type protein. This suggests that this could be a possible potential candidate for the treatment of Acute Lymphoblastic Leukaemia (ALL) with less induced side effects.

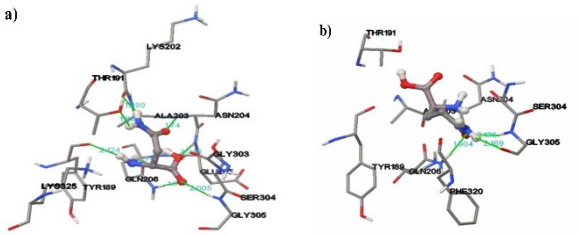


Figure (1): Docking results of mutant protein Y306L a. with L- Asparagine; b. with L-Glutamine.

**References:**

1. Labrou NE, Papageorgiou AC, Avramis VI. Structure-function relationships and clinical applications of L-asparaginases. Curr Med Chem
2. 2010;17(20):2183-2195.
3. Ramya LN, Mukesh Doble, Rekha PB, and Pulicherla KK. In silico Engineering of L-Asparaginase to Have Reduced Glutaminase Side Activity for Effective Treatment of Acute Lymphoblastic Leukemia. J Pediatr Hematol Oncol 2011; 33:617-621.
4. Kumar S, Dasu VV, Pakshirajan K. Localization and production of novel L-asparaginase from Pectobacterium carotovorum MTCC 1428. Process Biochemistry 2010; 45:223-229.

***Keywords***: *L-asparaginase, acute lymphoblastic leukaemia (ALL), docking, molecular dynamics, site-directed mutagenesis.*

**BCI 06**

# Identification of MHC class-II epitopes in Chandipura Virus G-protein

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Chandipura virus (CHPV) is negative sense RNA virus belonging to the genus *Vesiculovirus* of family *Rhabdoviridae.* Since its emergence in 2003, Andhra Pradesh outbreak, the virus has been identified as a cause of acute encephalitis in pediatric population from different states of India especially Gujarat, Maharashtra, Andhra Pradesh, Telangana, Bihar and Odisha. Considering the acute nature of disease and increasing spread to newer areas, promising preventive measures should be developed. The G-protein is the surface protein of CHPV that interacts with the host immune system. We have identified a conserved neutralizing epitope in the G-protein of CHPV by developing and using neutralizing MAb to G-protein of CHPV. The central event in the generation immune response is the activation and clonal expansion of T-cells. $CD4^+$ T cells plays pivotal role in the protective immune response against different infectious agents. Thus, to further investigate the antigenicity, an immuno-informatics approach was applied to screen potential MHC class-II-restricted epitopes that can activate the immune cells. The MHC class-II epitopes for G-protein were predicted based on different MHC class-II alleles predominant in human population of Gujarat and Telangana/Andhra Pradesh, regions of India which witnessed continuous CHPV activity since 2003. online IEDB tools have been used for prediction of MHC class-II epitopes. The predicted epitopes were further analysed using stringent percentile cut-off of ≤5 and ability to get presented by maximum number of alleles from outbreak areas. In this study we have identified three MHC class-II restricted epitopes in the G-protein of CHPV. One of these epitopes is also a part of a neutralizing B-cell epitope. This is an important finding that may hold a promise towards the development of protective targets against CHPV infection.

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**MR 01**

# Antidiabetic, antihyperlipidemic and antioxident activities of *Stachytarpheta urticifolia* Salisb (sims) methanol leaf extract in streptozotocin-induced types I and type II diabetic rats

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To evaluate the antidiabetic, antihyperlipidemic and Antioxident activities of Stachytarpheta urticifolia Salisb (sims). Wistar rats were divided into nine groups of six animals each, and 40 mg/kg of streptozotocin or streptozotocin + nicotinamide was administered intraperitonially to induce types I and II diabetes. Those with blood glucose levels > 190 ± 8 mg/dl were administered the methanol leaf extract of Stachyterpheta urticifolia Salisb (sims) (MESU, 100 or 200 mg/kg, p.o.) or positive control for 21 days. Blood glucose, lipid profile and oxidative stress markers were evaluated.

***Keywords:*** *antidiabetic, antihyperlipidemic, antioxidant, Stachytarpheta urticifolia Salisb (sims)*

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**MR 02**

# Unraveling the link between molecular confinement and enzyme stability in bacterial microcompartments

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Bacterial microcompartments are proteinaceous membrane less organelles like structures found in many species of bacteria that span close to 19 different phyla. These structures are formed by self-assembly of thousands of protein sub-units encoded by genes belonging to a single operon. They perform various metabolic functions contributing to global carbon fixation and bacterial pathogenicity. Propanediol-Utilization Microcompartments, found in *Salmonella enterica* provide selective advantage to the bacteria under carbon deficient gut microenvironment by enabling them to utilize 1,2-propanediol as a carbon source. The *pdu-operon* encodes for Pdu-shell proteins and Pdu-enzymes. Pdu-shell proteins tile edge to edge and form the outer coat of the microcompartment and Pdu-enzymes are encapsulated within. The aim of our work is to understand the effect of volume and space confinement due to the encapsulation, on the thermal stability of Pdu-enzymes. Comparative enzyme assay using the microcompartment and one of its purified enzymes PduCDE, shows that the microcompartment is thermally more stable than the purified enzyme. This observation is consistent with our biophysical results which suggest that encapsulation of enzyme within the microcompartment provides them thermal stability. In order to understand the contribution of shell proteins to the thermal stability of the enzymes, we study the activity of PduCDE in the absence and presence of the major shell protein PduBB'. We observe an enhanced enzyme activity of PduCDE in the presence of the shell protein PduBB'. Biophysical studies show that the shell protein PduBB' not only provides interaction based thermal stability to the enzyme but also acts like a chaperon, and prevents the aggregation of the enzyme under sub-denaturing temperature. Besides, bioinformatics studies reveal the presence of intrinsically disordered regions among the Pdu-proteins. Careful analysis of these disordered regions indicates their role in protein-protein interactions, which are important the biogenesis of the microcompartments. We propose that the disordered regions in the Propanediol-Utilization Microcompartments provide flexible backbone and help Pdu-proteins in binding with their protein partners.

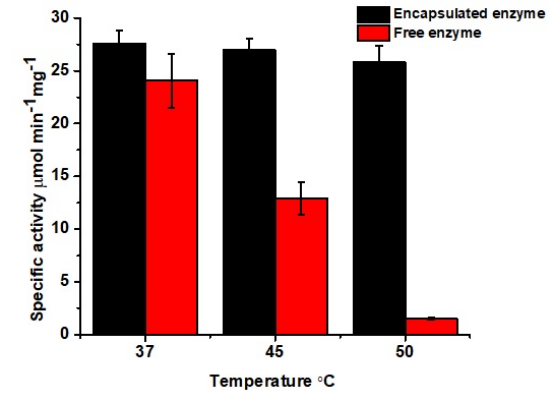


Figure (1):

**References:**
1) Kerfeld, Cheryl A., Sabine Heinhorst, and Gordon C. Cannon. "Bacterial microcompartments." *Annual review of microbiology*64 (2010).
2) Havemann, Gregory D., Edith M. Sampson, and Thomas A. Bobik. "PduA is a shell protein of polyhedral organelles involved in coenzyme B12-dependent degradation of 1, 2-propanediol in Salmonella enterica serovar Typhimurium LT2." *Journal of bacteriology* 184.5 (2002): 1253-1261.

***Keywords***: *microcompartments, propanediol*

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**MR 03**

# Identification of targets in *Synechococcus* PCC7942 for improved biofuel precursor production

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*Synechococcus* PCC7942 has recently been considered potential candidate for engineering with the objective to improve its ability to synthesize biofuel precursors and other value-added products. Engineering such a strain requires a detailed understanding of the key metabolic pathways through which flux is transferred and the enzymes that orchestrate the interconversion of metabolites in these pathways. Rich genome-wide gene expression data under variety of conditions are now becoming available for the model cyanobacterial species *Synechocystis* sp. PCC6803, which is phylogenetically close to the *Synechococcus* PCC 7942. Using these data and the existing metabolic flux model of the same species, in this study, we contrast the levels of flux through various key pathways such as glycolysis, TCA cycle and the regulation of the metabolic enzymes involved. By appropriately combining the flux levels and regulation levels, we identify the (metabolic) genes that could be considered targets for engineering and thereby facilitating increase of flux to pathways culminating in the biofuel precursors such as 1-Butanol. Further, assessment of the dynamics of the gene expression for identification of transcription factors that may be regulating these metabolic enzymes will be presented.

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**MR 04**

# A study to cross-link stress resistance and metabolic pathways

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Metabolic pathways play an important role in the cell's overall behaviour. It is known that during stress, the cell modulates the expression of its metabolic genes (1). We aim to employ a systems biology approach to integrate the data obtained from genomic, transcriptomic and metabolic studies into a mathematical model which can simulate the biological processes taking place in a cell.

A deinococcal regulator was introduced into *Escherichia coli* (2). This recombinant strain (MG-1558) showed considerable acid stress tolerance as compared to the wild-type strain (MG-PR) (Fig. 1). These cultures were grown in a bioreactor under stress and non-stress conditions to estimate their growth parameters, the rate of secreted metabolites and substrate uptake.

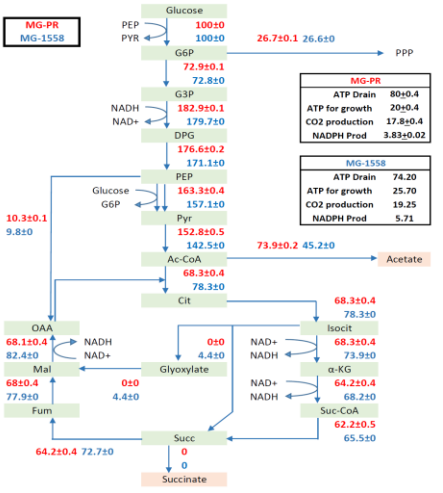


Figure (1): Growth profile of MG-PR and MG-1558 at different pH

This data was used to simulate the overall flux distribution pattern through the central carbon metabolic pathway using the steady state gene expression simulator (Fig. 2). Certain key metabolic nodes were identified that function differently in a stress resistant strain as compared to a stress-sensitive strain.

Understanding the regulatory networks of key metabolic pathways that are differentially expressed in a resistant organism can be used to select novel potential targets for engineering of robust industrial strains.

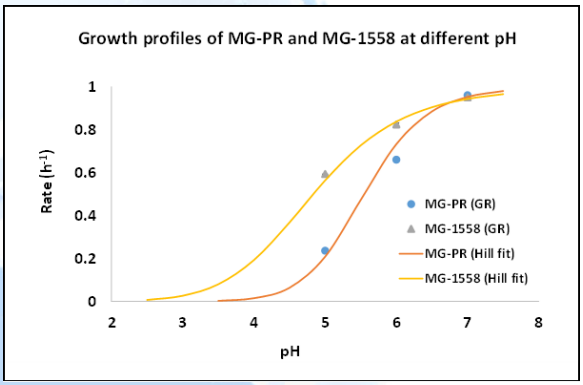


Figure (2): Metabolic flux map of MG-PR and MG-1558 grown in M9 media at pH 5.0

**References:**

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***Keywords***: *metabolic engineering, metabolic flux analysis, stress resistance, systems Biology*

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**MR 05**

# A steady state model for simulation and prediction of cell membrane and peptide binding mechanisms with experimental validation

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Anti Microbial Peptides (AMPs) are being designed and used in place of antibiotics to combat drug resistance (Baltzer & Brown, 2011). An AMP binds to the membrane of the organism and undergoes changes in conformation and aggregation state to enable killing action and there have been ongoing studies to elucidate the exact mechanism of binding. The nature of binding can be aggregating or non-aggregating, with high or low cooperativity, at single or multiple sites or with high or low affinity. In this study, we present a steady state model that simulates the binding between an AMP and a membrane to predict the mechanism of binding using two variables as input, the Hill coefficient and Half saturation constant from the cell death response of the action of AMP on the host organism. The model has found to predict accurately aggregation, number of sites, cooperativity and strength of binding for experiments found in literature. This model can be used to predict the mode of action for any cell membrane and peptide binding irrespective of the type of the organism and hence can generate hypotheses for experimental verification. We have verified the predictions with experiments from literature and predicted the mechanism for a set of newly designed AMPs with high sequence similarity to Myeloid Antimicrobial Peptide (MAP) family with enhanced killing capacity.

Figure1 depicts the action of an AMP on the cell membrane resulting in its killing action. The killing response is plotted as Cell (microbe) death percentage versus the peptide concentration. The parameters nH and K0.5 are estimated using Hill's Equation. The same parameters are predicted using different mechanisms for a given AMP death rate response curve as shown in Table 1. The mechanism which predicts (nH, K0.5) pair that has the least MSE compared to the one determined by the actually measured death rate response is considered to be the mode of action of the peptide.

Table (1): Different mechanisms are used to predict the nH and K0.5 for Melittin binding to a cell membrane. The prediction with the least MSE compared to the experimentally observed parameters is Oligomerization. Melittin is known to tetramerize before binding to the cell membrane thereby increasing its efficacy.

| Melittin hRBCs (4.4, 2.86) | Only Binding | Multiple site No Cooperativity | Multiple SItes Cooperativity | Aggregation Cooperativity + Multiple sites | Oligomerization Cooperativity |
|---|---|---|---|---|---|
| MSE | 3.89 | 3.43 | 2.64 | 2.89 | 0.11 |
| nH | 1 | 1 | 1.77 | 3.93 | 4.36 |
| K0.5 | 1 | 2.5 | 2.93 | 0.01 | 2.76 |
| KD | 1.00E+00 | 1.00E+01 | 1.50E+01 | 1.00E+00 | 2.5 |
| Num Sites | 1 | 2 | 2 | 3 | 2 |
| Cooperativity | NA | NA | 20 | 20 | 50 |
| Aggr | No | No | No | 4 | No |
| Olig | No | No | No | No | 4 |

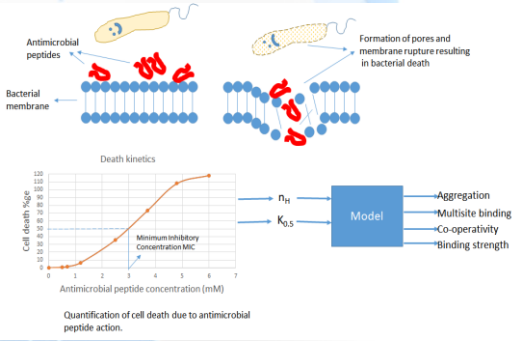


Figure (1): Prediction of mechanism of action of AMP

**References:**
1. Baltzer, S. A., & Brown, M. H. Antimicrobial peptides: promising alternatives to conventional antibiotics. J Mol Microbiol Biotechnol. 2011, 20(4): 228–235.

***Keywords**: antimicrobial peptides, mode of action.*

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