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भारतीय प्रौद्योगिकी संस्थान धारवाड
Indian Institute of Technology Dharwad

SPECTROMICS - 2026

SPECTROMETRY-INTEGRATED OMICS IN HEALTH AND DISEASE

A National Conference Organized by Dept. of Biosciences & Bioengineering,

Indian Institute of Technology Dharwad, Karnataka, India.

Abstracts & Annotations

SPECTROMICS - 2026

SPECTROMETRY-INTEGRATED OMICS IN HEALTH AND DISEASE

16th –17th January

Welcome Note from the Organizers

On behalf of the organizing committee, we are delighted to welcome you to the SPECTROMICS 2026 Conference. Over the coming days, you will have the opportunity to engage in stimulating discussions, explore ground breaking research, and forge new collaborations. We have curated an exciting program and networking events designed to inspire innovation and foster knowledge exchange. Whether you are a seasoned expert or new to the field, the vibrant mix of invited speakers, student presenters, and local participants promises a dynamic and enriching experience for all. Some of the major conference highlights are listed below

- Invited Speakers: Over 20 renowned speakers from across the country will present on cutting-edge topics in spectrometry and omics technologies.
- Poster Presentations: More than 40 poster presentations will showcase ongoing research, innovative methodologies, and impactful findings from a diverse group of participants.
- Student Presentations: Short presentations will provide a platform for young researchers to share their work and receive valuable feedback from expert audiences.
- Pre-Conference Workshop: A workshop focused on "Chemometrics: Empowering Scientific, Industrial, and Regulatory Decisions Through Intelligent Data Analytics" organized by Science4U will be held prior to the main conference.
- Connecting minds: The conference will welcome close to 150 delegates from local institutes interested in exploring opportunities for collaboration in education, research, and community engagement.

We take this opportunity to acknowledge the financial support from Anusandhan National Research Foundation **(ANRF)** and Department of Biotechnology **(DBT)**. In addition, generous contributions from our sponsors Oxford Instruments, LabIndia, Horiba, Thermo Scientific and The Dharwad Research and Technology Incubator Foundation (dhaRti) are gratefully acknowledged. We would also like to extend my sincere appreciation to all the faculty members, staff, student volunteers and administration of IIT DHARWAD for their dedication, teamwork, and tireless efforts in organizing this conference. Their collective support has been the backbone of this event. Let us use this opportunity to exchange ideas, build collaborations, and contribute collectively to the advancement of omics field for health sciences.

"Wishing you all a fruitful and inspiring conference experience at IIT DHARWAD".

Dr. Surya Pratap Singh,
BSBE Dept., IIT Dharwad

Dr. Nilkamal Mahanta
Chemistry Dept., IIT Dharwad

Dr. Badri Nath Dubey
BSBE Dept., IIT Dharwad

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Microfabricated Devices and Interfaces for Biomarker Detection & Liver Injury Modelling

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We will describe an integrated polydimethylsiloxane microfluidic device for Aβ1–42detection and it offered very reliable measurements. The SERS technique was used for this device to afford noise-free measurements, with excellent limit-of-detection values approaching 10^{-18}-10^{-15} M when tested with simulated cerebrospinal fluid. In another approach, we microfabricated a membrane-free liver-on-a-chip interface to create a native-like 3D microenvironment for an ensemble of HepG2, NIH-3T3, and HUVEC, in a hydrogel. Functional validation was confirmed from albumin and urea secretion, with the interface exhibiting sustained CYP1A1 enzyme activity. This sealed device has the potential for predicting drug-induced liver injury, and it could be developed as a useful platform for disease modelling.

Next-Generation Proteomics: Advances in Technologies and Computational Solutions

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Proteomics has witnessed transformative advancements in recent years, with high-resolution mass spectrometry (MS), targeted approaches, and powerful computational tools propelling large-scale analysis of protein expression, modifications, and interactions. These innovations, combined with databases and interactive platforms, have broadened the scope of proteomics across diverse fields, from basic research to clinical applications. Despite these advancements, the full potential of these technologies remains largely untapped in clinical and biological applications. This talk will highlight key developments in MS-based proteomics, focusing on advancements in instrumentation, workflows, and data acquisition strategies such as Data-dependent Acquisition (DDA) versus Data-independent Acquisition (DIA). A comparison between discovery and targeted proteomics will be discussed, alongside non-MS-based approaches, including protein arrays and label-free Surface Plasmon Resonance (SPR) and Biolayer Interferometry (BLI) will also be briefly discussed. We will also explore emerging proteomics applications, including single-cell proteomics and cell surface proteomics, aimed at understanding the functional crosstalk between cells and advancing our knowledge of disease biology. Innovative platforms like Proximity Extension Assay (PEA) and SomaScan, along with the Proteograph platform, will be presented as tools for plasma proteomics. In the realm of software and database development, we will showcase our recent work on tools such as AlphaCross-XL for identifying protein cross-linking, and BrainProt, a comprehensive resource for the Human Brain Proteome Project, which integrates proteomic and transcriptomic data with clinical insights into brain diseases. BrainProt offers cutting-edge analysis tools to accelerate biomarker discovery and drug development for neurological disorders. Additionally, a novel computational pipeline for predicting the druggability of human proteins will be discussed, using machine learning models like Random Forest and XGBoost.

Spectroscopic Innovations Leading Translational Research

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Recent advances in chemical and optical sciences have enabled a new way in biomedical diagnostics by coupling molecular-level spectroscopic precision with the computational power of artificial intelligence. This talk highlights the outcomes of our laboratory on machine learning-enabled fluorescence and photoacoustic spectroscopy in observing protein alterations, and early detection and monitoring of diseases such as breast cancer, oral cancer, colorectal cancer, diabetes, and neurodegenerative disorders. Our research demonstrates that photoacoustic spectroscopy provides sensitive insights into biochemical and structural alterations within tissues, while fluorescence spectroscopy captures dynamic molecular changes associated with protein conformational shifts and mitochondrial dysfunction. By employing data-driven methods such as support vector machines, generalised linear models, and feature-selection algorithms, we achieve high sensitivity and specificity in differentiating healthy and diseased tissues across preclinical and translational models. Selected studies explore photoacoustic signal-based classification of breast tumour progression in vivo, oral cancer identification through spectral-textural analysis, and dual-modality fluorescence–photoacoustic spectroscopy for mapping metabolic and vascular biomarkers. Further, our work on glycated protein autofluorescence provides promising diagnostic markers for diabetes and systemic oxidative stress. The synergy between optical spectroscopy and AI opens opportunities for developing non-invasive, label-free, and real-time diagnostic tools, bridging fundamental chemistry with clinical applications. This integrative framework positions multimodal spectroscopic diagnostics as a cornerstone of next-generation chemical–biomedical innovation, aiming for precision disease detection and personalised monitoring.

Fluorescent Quantum Clusters: Towards Biomedical Properties

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The research on functionalized metal nano-materials is showing the enormous concern due to their noble properties depends on the alteration in size, shape, and the material itself. Among the metal nano-particles, gold nanoparticles (Au NPs) are popular for biomedical applications because of their simple and fast synthesis; excellent biocompatibility using appropriate ligands; bio-conjugation; shape-, size-, and surrounding chemical-environment dependent tuneable optoelectronic properties; suitability as a platform for multifunctionalization with a wide range of biological ligands. Recently, growing interest has been mainly focused on noble gold quantum clusters (Au QCs) due to their size-dependent optical properties, better water solubility, biocompatibility, and low toxicity. In my talk, the synthesis of Au NPs and Au QCs using the various ligands that act as both reducing and capping agents will be discussed. The influence of HAuCl4/ligand concentration, temperature, and pH, which shows the crucial factors in the modulation of the nucleation and growth kinetics of the reaction, and consequently, in guiding the size and morphology of as-synthesised Au NPs, will be also presented. Further the synthesis and fundamental understanding of Au QCs which is originated from Au NPs will be discussed under different pH conditions. The biomedical and sensing applications of the as-synthesized Au QCs will be shown on the basis of an aggregation- induced fluorescence quenching mechanism.

Development of an ultra-sensitive laser stimulated fluorescence system for simultaneous detection of amino acids

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We developed and validated an ultra-sensitive detection system based on high-performance liquid chromatography combined with laser-stimulated fluorescence. This setup allows us to detect 20 different amino acids simultaneously after derivatizing them with dansyl chloride. Dansyl chloride was used as a derivatizing agent, and key derivatization parameters, such as reaction time and temperature, were optimized to enhance sensitivity and reproducibility. Most amino acids showed a relative standard deviation below 5%, demonstrating that the method is highly reliable. It was also extremely sensitive, with detection limits ranging from 4.32 to 85.34 femtomoles, and it produced strong linear responses, with R^2 values above 0.98 for all amino acids. We further tested the system using human serum samples and successfully identified the eluted amino acids. Overall, this method offers a powerful, user-friendly, and cost-effective approach for analyzing amino acids in various body fluids. Its high sensitivity and reliability make it a valuable tool for diagnosing and managing disorders linked to abnormal amino acid levels.

Human platelet activation probed by micro-Raman Spectroscopy

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The study of blood components at the single-cell level is essential for understanding their structural and functional dynamics in both healthy and disease conditions. Raman Tweezers, an integration of optical trapping and Raman spectroscopy, offer a powerful platform for characterising individual cells in their native aqueous environment. This technique enables the acquisition of Raman spectral fingerprints from red blood cells (RBCs), revealing haemoglobin conformational changes, oxygenation states, and related biochemical variations. It enables a detailed examination of platelets, where spectral markers of membrane proteins, lipids, and intracellular biomolecules can be identified, providing insights into biochemical signatures associated with platelet activation.

A key application of this technology is the study of storage-induced changes in blood components, which directly impact the quality of transfusions. During storage, RBCs and platelets undergo progressive biochemical and structural alterations, collectively referred to as storage lesions, which compromise their viability and function. Raman Tweezers enable molecular-level monitoring of these degradation processes with single-cell precision, facilitating early detection of alterations. Overall, this approach offers significant potential for improving blood component characterisation, refining storage protocols, extending shelf-life, and ultimately enhancing transfusion safety.

Raman Spectromics: Explorations in Disease Diagnosis

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Optical theranostics alternatively or interchangeably also referred to as optical pathology, optical biopsy, spectral diagnosis describe applications of spectroscopic and/or optical based methods in disease diagnosis and management. Conventionally, diseases are diagnosed by clinical examination followed by relevant biochemical/microbiological/pathological/imaging examinations, which rely on symptomatic manifestations, often lead to late diagnosis in turn poor prognosis. Since biochemical changes precede morphological/symptomatic changes, optical spectroscopies which are sensitive alterations chemical compositions are emerging as potential alternatives/adjuncts. Major attributes of these methods are: less time consuming, no external labelling or sample processing, more objective, and most importantly in vivo/in situ on line diagnosis. Laser-induced-fluorescence, FTIR, Raman and diffuse reflectance are some of the well-known optical methods. The present talk discusses our studies on applications of Raman spectroscopy tools towards non-cancerous disease diagnosis and therapeutic monitoring.

Morpho-Molecular Microscopy: Advancing Cancer Diagnosis and Intraoperative Margin Assessment

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Tumorigenesis is a complex process that involves dramatic changes in the morphological, molecular, and genetic makeup of cells as they transform from normal to malignant. Raman spectroscopy offers the ability to study live cells without the use of external contrast agents. However, the clinical application of spontaneous Raman imaging is limited by its slow speed and low sensitivity. To overcome these challenges, we developed a novel technique known as morpho-molecular microscopy (3M), which allows for simultaneous measurement of both morphological and biochemical characteristics. Our 3M system draws on the combined strength of quantitative phase imaging - to probe the morphological features- with Raman microscopy that provides molecular fingerprinting characteristics. This talk will discuss the use of the 3M system in live-cell imaging and its applications in leukaemia diagnosis. The other focal point of this talk will highlight our recent clinical translational efforts in intraoperative breast cancer detection using another morpho-molecular approach.

Spin-selective charge transfer-SERS-based label-free enantioselective discrimination of chiral molecules on Ag nanoparticles decorated Ni nanorod arrays

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Enantioselective discrimination is critical in several fields, particularly pharmaceutics and clinical drug research. Chiral molecules possess unique charge transfer properties, showing an enantioselective preference for the electron spin orientation when interacting with the magnetic surface. Here, we developed spin-selective charge transfer (SSCT) based label-free surface-enhanced Raman scattering (SERS) achiral magnetic substrates for enantioselective discrimination of chiral molecules without creating asymmetric chiral adsorption sites. The e-beam-based glancing angle deposition (GLAD) technique was utilized to fabricate the achiral magnetic surface-enhanced Raman scattering (SERS) substrates by decorating Ag nanoparticles on Ni nanorods. SERS spectroscopy was carried out on significant enantiomers, including cystine, alanine, and DOPA (l-3-(3,4-dihydroxyphenyl) alanine). A powerful external electromagnet manipulated the magnetic substrate's spin polarisation by altering the magnetic field's direction. Subsequently, SERS spectra were acquired. Based on the direction of the magnetic field, there is a complementary variation in the intensities of SERS spectra of the enantiomers. The SSCT process between molecule-metal complexes synergized with the external magnetic field direction to control the electron spin, leading to SERS-based enantioselective discrimination. This label-free, easy, yet practical approach offers a characteristic paradigm shift from the recent complex approaches for chiral detection and separation.

Nanosculptured Plasmonic Thin Films Enhanced Spectroscopic Sensors for Diagnostics

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Nanosculptured plasmonic thin films (nSTFs) are porous columnar films supporting localized surface plasmon resonance (LSPR). Ultra-high plasmonic field enhancements in the vicinity of these nSTFs provide an avenue for huge enhancement of spectroscopic signals (fluorescence/Raman) of molecules placed close to the surface. This enhancement is called surface-enhanced- fluorescence (SEF)-Raman spectroscopy (SERS). In this talk, I will introduce the basics of surface plasmon-based spectroscopic enhancement and then delve into the SEF and SERS based biosensor studies performed in my research group. In particular, label free, yet SEF based sensing of HbA1c will be disucssed, while the SERS based sensor studies will comprise of machine learning enabled classification of respiratory viruses in clinical nasopharyngeal samples, and detection of a traumatic brain injury biomarker.

Magnetoelectrically and Photo-Induced Surface-Enhanced Raman Signal Amplification for Next-Generation Ultrasensitive Molecular Recognition

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Traditional Surface-Enhanced Raman Spectroscopy (SERS) is limited by the lack of controlled molecular interactions on plasmonic surfaces, which hampers sensitivity, particularly for analytes with inherently weak Raman activity. Earlier strategies, such as Photoinduced Enhanced Raman Spectroscopy (PIERS), sought to amplify the chemical enhancement mechanism by leveraging electron dynamics across a metal-semiconductor junction. PIERS typically involved the synthesis of semiconductor substrates where UV pre-irradiation created oxygen vacancy defects to facilitate electron transfer to plasmonic nanoparticles. However, reliance on UV light for pre-activation can be a constraint. To overcome this, we introduce Magnetoelectrically Induced Surface-Enhanced Raman Signal Amplification (MIERS), a technique that replaces non-selective UV pre-irradiation with continuous, in-situ magnetic field modulation. The MIERS platform utilizes an Advanced Magnetoelectric Nanostructure (AMEN), fabricated via ultrasonic spray pyrolysis, featuring a cobalt ferrite (CFO) nanorod embedded within a barium titanate (BTO) hollow nanosphere, surface-modified with plasmonic silver nanoparticles. In this intricate design, the application of an external magnetic field induces strain in the CFO-BTO heterostructure, generating localized electric dipoles and free charge carriers through the magnetoelectric effect. The resulting prolonged charge-carrier lifetime, coupled with a Schottky barrier at the metal–ME interface that suppresses charge back-transfer, ensures a unidirectional flow of charge to the analyte molecule. Critically, MIERS demonstrated enhancement factors up three orders of magnitude higher than conventional SERS, substantially surpassing the typical ~50-fold amplification observed in PIERS. These findings establish MIERS as a unique, versatile, and high-impact platform for precise analytical and biomedical sensing, enabling continuous and controllable chemical enhancement.

Next-Gen SERS Platforms for Ultrasensitive Detection of Chemicals and Biomolecules

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Surface-enhanced Raman spectroscopy (SERS)[1] has gained significant attention in the scientific and industrial communities due to its ability to detect a broad range of analytes, including chemical contaminants, biomolecules, food-borne pathogens, pharmaceutical drugs, and electrochemical species, with additional advantages such as portability and rapidity. Owing to its high sensitivity and simplicity, this vibrational spectroscopic technique has been widely applied in bioanalysis, environmental monitoring, and food safety. One of the major advantages of Raman-based techniques is their capability to provide fingerprint information with sharp Raman peaks, making SERS a suitable approach for the identification of multiple analytes in real-world samples.

In this talk, the fundamentals of SERS, various fabrication methods for plasmonic nanostructures (SERS substrates), and applications will be discussed. Particularly, the potential applications of SERS include: i) detection of toxic environmental contaminants such as microplastics and perfluoroalkyl substances (PFAS),[2] ii) detection of hazardous dyes in food samples,[3] and iii) applications of SERS in disease diagnosis and bioanalysis.[4]

Decoding ALS through Integrated-Omics Approaches: Insights from Gut Microbiota and NMR-Based Metabolic Signatures

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Amyotrophic Lateral Sclerosis (ALS) is a progressive and fatal neurodegenerative disorder characterized by the relentless loss of motor neurons. Although extensive research is underway, available treatments remain limited, and the disease's underlying mechanisms are still not fully understood. Increasing evidence indicates that gut dysbiosis, immune dysregulation, and metabolic disturbances may contribute significantly to ALS pathogenesis. To investigate these connections, we conducted an integrative multi-omics, case–control study combining shotgun metagenomics with ^{1}H Nuclear Magnetic Resonance(NMR)-based metabolomics using serum and stool samples from ALS patients and their household controls, who shared comparable diets and environments. Our findings revealed distinct alterations in the gut microbiome of individuals with ALS, including increased abundances of Bifidobacterium, Lactobacillus, and Enterococcus, while Lactiplantibacillus and Klebsiella were more prevalent in household controls. Metabolomic profiling identified 15 significantly altered metabolites—six in stool and nine in serum—including key short-chain fatty acids (butyrate, propionate), branched- chain amino acids (isoleucine, leucine), and intermediates of energy metabolism. Receiver operating characteristic (ROC) analysis highlighted isoleucine (AUC = 0.83), butyrate (AUC= 0.798), and citrate (AUC = 0.719) as candidate biomarkers with diagnostic potential. Pathway enrichment analysis indicated disruptions in the glucose–alanine cycle, urea cycle, ammonia recycling, and the Warburg effect, emphasizing the involvement of mitochondrial dysfunction and neuroinflammatory processes in ALS. Overall, this study underscores a complex interplay between the gut microbiome and host metabolic pathways, offering new insights into ALS biology.

Mapping the Metabolic Code of the Human Brain: Insights from Gliomas, Healthy Function, and Neonatal HIE

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Metabolic state is a critical determinant of cellular identity, energy regulation, and disease progression in the human brain. Our research integrates advanced in vivo ^{1}H magnetic resonance spectroscopy (MRS), ex vivo NMR metabolomics, and machine learning to systematically map metabolic remodelling across brain tumours, healthy neurological systems, and neonatal hypoxia-ischemic encephalopathy (HIE). Using high-resolution MRS in healthy subjects, we demonstrate that neurochemical distribution across brain regions is inherently heterogeneous, reflecting region-specific functional specialisation and offering a quantitative basis for understanding intrinsic brain physiology.

In gliomas, we combine patient MRS profiles with genetically defined cell-line models to interrogate subtype-specific oncogenic reprogramming. Leveraging precise quantification of 2-hydroxyglutarate (2-HG), we define distinct metabolic signatures of IDH-mutant gliomas and reveal rewired nutrient utilization patterns. Parallel consumption-release (CoRe)metabolic flux analyses show that while cancer types share convergent bioenergetic features, each lineage exhibits unique uptake and secretion kinetics shaped by its genetic and microenvironmental context.

Extending this framework to acute brain injury, we implement rapid plasma metabolomics in neonates to identify early markers of HIE within hours of birth. When integrated with machine- learning classifiers, these metabolic signatures enable highly accurate differentiation of HIE from non-HIE neonates, presenting a clinical pathway for timely neuroprotective interventions. Together, these complementary studies establish a multimodal metabolic mapping platform that reveals disease-specific biochemical vulnerabilities, supports precision neuro-oncology, and advances quantitative neurodiagnostics for both developmental and acquired brain disorders.

Cracking the Code of Oxidative Stress: How We Track Tiny Clues in Urine

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Oxidative stress is like rust forming inside our bodies it quietly damages cells and contributes to many health problems. But how do we detect it before it causes harm? The answer lies in tiny chemical clues hidden in something as simple as urine. In this talk, we'll explore how advanced analytical tools help us uncover these clues. Using a highly sensitive technique called liquid chromatography–mass spectrometry, we can measure key intermediate molecules as indicators of oxidative stress. Our method is precise, reliable, and capable of detecting these molecules at incredibly low levels. This breakthrough opens doors to better monitoring of health and disease, making invisible processes visible and actionable. Join us to see how cutting-edge science is transforming the way we understand and track oxidative stress.

Nanomaterials based Portable sensors for protein biomarkers of Cancer

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Cancer is the second most leading cause of deaths across the globe, and its incidence is increasing with each passing day. The survival rate and the treatment outcomes of almost all types of cancer can be significantly improved if they are diagnosed at an early stage. While the delayed diagnosis can be attributed to multi-dimensional factors including low awareness among the population, no/mild symptoms at early stage, costly and lab-based tests, development of point-of-care devices which are efficient and portable for detection of specific markers of each cancer types, is certainly believed to aid in the early-stage diagnosis of the disease. This talk will describe in detail the development of 2-port resistive sensor devices for a few specific markers of prostate and ovarian cancers. These markers would include clinical markers like CA125 and PSA as well as a few novel markers like PCA3, SPINK1, and PCAT14. The device structure, intricacies involved in the development of the device and interesting observations made during the device characterizations would be discussed.

Developing Raman Spectroscopy for Drug Discovery and Diagnostics

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The talk is going to dwell in the realms of discovering the therapeutically important protein structure using Raman spectroscopy and molecular dynamics simulations using noble metal nanoparticles. X-ray crystallography of protein crystals is the gold standard for determining the structure of proteins, and recently, cryo-EM has made it easy to determine the structures. Even with large developments in this field, there are many proteins for which structures are difficult to determine. We in our group have worked with such proteins or proteins where the structures exist to understand the protein structure function in their physiological conditions. We have been able to use this to do drug screening and diagnostics. The talk will elucidate this with various examples from our group.

Lipidomic changes in drug-naive/drug-free schizophrenia patients compared to healthy controls

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Schizophrenia (SCZ) lacks reliable biomarkers for early detection, as current diagnosis depends on subjective clinical evaluation. The study aimed to characterize lipid alterations in schizophrenia. In this prospective observational study, extracellular vesicles (EVs) were isolated by polyethylene glycol precipitation method and validated. Lipids extracted from plasma samples (n = 104; 52 SCZ and 52 controls) by Bligh and Dyer method and quantified using UPLC–MS/MS. Data were analyzed by using metaboanalyst version 6.0. Extracellular vesicle concentration was higher while size was significantly smaller in SCZ. Multivariate lipidomics (PLS-DA) revealed distinct lipids cluster, phosphatidic acid (PA 18:0/18:2), phosphatidylglycerols [PG 18:0/18:2, PG 18:0/18:1, PG 18:1/18:1], phosphatidylethanolamine (PE 18:0/20:4), phosphatidylserine (PS 18:0/18:0), sphingomyelins [SM d18:1/14:0, SM d18:1/16:1, SM d18:1/18:1, SM d18:1/18:2, SM d18:1/18:3], and hexosylceramides [HexCer d18:1/12:0, HexCer d18:1/18:1, HexCer d18:1/18:2, HexCer d18:1/20:1] as top discriminant lipids (VIP > 1). Volcano analysis identified 52 significantly altered lipids, and 17 showed good diagnostic performance (AUC > 0.70). Enrichment analysis suggested disrupted glycerophospholipid metabolism. The study confirms EVs carry distinct lipidomic signatures, particularly involving glycerophospholipid metabolism. Several lipids demonstrated good diagnostic potential, suggesting EV-lipid profiles aid in early detection of the disease.
Keywords: Extracellular vesicles, Lipidomics, Schizophrenia, Biomarker.

Stokes Vector-Based Second Harmonic Generation Microscopy for Biomedical Applications

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A Stokes polarimeter was build using four-channel photon counting detectors and integrated with second harmonic generation (SHG) microscopy for characterizing polarization properties of light. The Stokes–Mueller-based polarization technique enables detailed characterization of both SH light and sample properties. This system allows for the simultaneous measurement of polarization states and key polarization parameters without requiring repeated image acquisition. Two-dimensional polarization imaging facilitates in-depth investigation of molecular orientation in targeted specimens such as collagen fibers, skeletal muscle fibers, and starch granules. Additionally, a four-channel Stokes–Mueller polarimetry system integrated with machine learning has been developed in linear optics for the classification and characterization of ductal carcinoma tissue. This instrument offers a cost-effective solution for quantitative polarimetry in microstructural analysis of breast tissue samples. Various polarization parameters are derived from Stokes–Mueller polarimetry; notably, under circularly polarized incident light, higher degree of polarization values are observed. Integrating Stokes vector- based polarimetry with microscopy and machine learning provides powerful insights for detailed microstructural analysis of tissues and holds significant potential as a diagnostic tool.

Pseudo-Natural Productsas a New Paradigm in Bioactive Compound Discovery: Explorations beyond the 'Natural Productome'

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New compound design hypotheses for the discovery of novel bioactive molecules remains an area of profound interest due to the ever-growing need for new drugs. The 'natural productome' has served as a rich source of drugs. However, they are often structurally complex and synthetically intractable, resulting in the need for new guiding design strategies to generate novel NP-like scaffolds. Pseudo-Natural product (PNP) hypothesis proposes to combine natural product scaffolds in a synthetically tractable way to design novel scaffolds which are unknown through biosynthetic pathways, offering new opportunities for bioactive compound discovery. This talk will detail the design, synthesis and biological evaluation of Indotropane as a novel class of PNPs for the discovery of two molecules with orthogonal bioactivity: (a) Myokinasib and Myokinasib-II as a potent and isoform-selective chemical probe for Myosin Light Chain Kinase-1 and; (b) indotropane as an antibacterial agent against Methicillin- and Vancomycin-resistant S. aureus (MRSA and VRSA).

Label-Free Molecular Diagnosis of Cancer Using Infrared Spectral Pathology

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Cancer remains one of the leading causes of disease-associated mortality worldwide [1]. Early detection substantially improves patient survival; however, identifying cancers at their earliest stages is challenging because most precancerous conditions are asymptomatic.

The current gold standard for cancer diagnosis is excision or punch biopsy followed by histopathological evaluation [2]. This method relies on tissue staining and morphological pattern recognition. Although indispensable in clinical practice, histopathology is often time-consuming, labor-intensive, and subject to inter-observer variability, which can limit its statistical confidence. Furthermore, the dyes and chemicals used for staining may exert cytotoxic effects and can perturb small metabolites within the tissue. These limitations underscore the need for a rapid, robust diagnostic approach capable of detecting molecular alterations associated with early disease.

Optical spectroscopic techniques, such as fluorescence spectroscopy, infrared spectroscopy, Raman spectroscopy, and their imaging modalities have emerged as powerful diagnostic tools in oncology. These methods can overcome many challenges posed by conventional diagnostic techniques, offering label-free, non-destructive, and highly sensitive biochemical assessment of tissues. Spectral diagnosis enables rapid and real-time characterization of disease progression by detecting variations in protein–protein, protein–lipid, and protein–nucleic-acid interactions, as well as conformational changes that occur across different cancer stages or grades [3].

In this context, I will emphasize the application of infrared spectroscopic imaging as a spectral pathology tool for cancer diagnosis. Recent advances in the differentiation and classification of various grades of lung fibrosis and oral cancer using infrared imaging will be specifically highlighted [4,5].

SPECTROMICS - 2026

SPECTROMETRY-INTEGRATED OMICS IN HEALTH AND DISEASE

16th –17th January

PLATFORM DIALOGUES

SPEC/26- 036

Digital Leptospira Microscopist: An AI-Enabled Imaging Framework for Automated Leptospira Detection and Analysis

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Leptospira, a pathogenic spirochete responsible for leptospirosis, remains a major zoonotic concern, yet delayed detection can result in severe outcomes. Conventional bright-field microscopy provides limited contrast for visualizing these thin, motile organisms, while dark-field and fluorescence imaging, though enhanced, remain subjective and operator dependent. To address these limitations, we introduce the Digital Leptospira Microscopist, an AI-assisted analytical framework that interprets microscopy-derived visual data using deep-learning-based image analysis. The system integrates high-contrast dark-field and fluorescence inputs and employs a YOLO-based detection model fine-tuned on laboratory-annotated images to differentiate leptospira structures from background noise. Automated detection and artifact suppression improve interpretive clarity and reduce diagnostic ambiguity. Additionally, the platform quantifies bacterial burden, morphological variability, and spatial distribution, generating structured reports with detection overlays and confidence metrics. Designed to complement laboratory workflows, this assistant enhances diagnostic consistency, reduces manual review, and supports reliable early evaluation of leptospiral infections in diverse clinical settings worldwide.

Keywords: Leptospira; deep learning; microscopy analysis; YOLO detection model.

SPEC/26- 037

Cylindrical Substrate-Assisted Droplet-Based SERS for Rapid and Efficient Detection of Toxic Dye in Market Samples

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Detection of low-concentration and diluted target analytes within specific hotspot regions is essential ultra-sensitive SERS analysis. However, achieving high reproducibility and sensitivity for SERS substrates remains a significant challenge. In this study, we present the fabrication of AgNPs assemblies on a novel cylindrical plasmonic Cu rod substrate, using a drop-casting method to construct colloidal-based droplet-SERS platforms. The cylindrical substrate exhibits sufficient hydrophobicity, confining the analyte to the tip of the SERS surface and preventing aqueous sample spreading. This design enabled the analysis of samples as small as 4 µL, without a drying step. Additionally, aligning the cylindrical substrates into a 3D-printed holder facilitated the production of an array for high-throughput analysis. This strategy demonstrated outstanding SERS performance, with a relative standard deviation of 8.6% and substrate reusability. Under optimized conditions, Rho-damine B, a carcinogenic dye, was detected at a low threshold of 1 nanomolar in aqueous and real-world samples.

Keywords: Surface enhanced Raman spectroscopy (SERS),Droplet SERS, Cylindrical substrate, Rhodamine

SPEC/26- 038

Spectromics-Driven Precision Diagnostics in Oral and Maxillofacial Pathology: Integrating Imaging, Histology and Omics for Next-Generation Disease Profiling

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Advances in mass spectrometry–based omics have opened transformative opportunities for precision diagnosis in Oral and Maxillofacial Pathology (OMFP). "Spectromics"—the convergence of high-resolution spectroscopic imaging, quantitative proteomics, metabolomics, and AI-augmented analytics—provides a powerful framework to decode the molecular architecture of oral diseases beyond conventional morphology. This study demonstrates the application of multimodal spectromics to correlate imaging, histopathology, and proteomic signatures in bone and soft-tissue lesions of the craniofacial complex. Using QTOF proteomics integrated with Cone-Beam CT and digital histomorphometry, we identify distinct spectral fingerprints differentiating benign osteogenic lesions from fibro-osseous pathologies, highlighting differential expression of collagen subtypes, non-collagenous matrix proteins, and osteogenic transcriptional regulators (RUNX2, SP7, and WNT/β-catenin pathway targets). Advanced spectral deconvolution further enables the mapping of biochemical gradients within lesions, revealing metabolic heterogeneity that remains invisible to light microscopy.

Our findings underscore the diagnostic and translational potential of spectromics in early lesion characterization, prognostic stratification, and identification of therapeutic targets. By bridging molecular data with diagnostic pathology, spectromics promises a paradigm shift toward mechanism-oriented, data-driven precision oral healthcare. This abstract advocates for incorporating spectromics into academic curricula, research workflows, and clinical decision- support systems in OMFP.

Keywords: Mass spectrometry, proteomics, precision diagnosis, oral & maxillofacial pathology

SPEC/26- 039

Decoding Oral Carcinogenesis usingSerum Raman Spectroscopy and Mass spectrometry-based Metabolomics

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Oral cancer remains a major global health challenge, with high morbidity and mortality largely resulting from diagnosis at advanced stages. This highlights the need for minimally invasive, rapid, and objective screening tools for early detection and timely intervention. Using the well-established hamster buccal pouch model of DMBA-induced oral carcinogenesis, weekly photographic monitoring over 14-weeks documented a clear transition of mucosa from normal-premalignant-malignant stages. In parallel, serum samples from DMBA-treated animals and age-matched controls were analysed using Raman spectroscopy (RS) and mass spectrometry (MS) to track biochemical and metabolic changes during disease progression. Serum RS detected early alterations, with PC-LDA showing distinct clustering from S0 to S4, and MCR-ALS revealing pronounced changes in protein and lipid profiles. MS profiling identified 2,618 metabolites, and PCA of control samples confirmed that the metabolic shifts in treated animals were DMBA-specific rather than age-related, supporting the RS observations. Significantly altered metabolites found were known to be associated with key processes in oral cancer development. Together, RS-MS approach provides valuable insights into biomolecular events underlying carcinogenesis. While MS offers high molecular specificity, its complexity limits routine use. In contrast, serum RS presents as an adjunct tool with strong potential for early oral cancer screening.

Keywords – Hamster buccal pouch model, Raman spectroscopy, Serum metabolomics, oral cancer screening

SPEC/26- 040

My Oralspectrometry: modular, offline, oral cancer research software

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My Oralspectrometry is a modular, offline-first application designed to simplify the interpretation of proteomics, metabolomics, and histology data for education in health and disease. The platform convertsroutine laboratory and clinical outputs into structured overlays, enabling learners to visualise omics information with clarity. Its design emphasizes fixed-axis scaling, intuitive navigation. By integrating computational workflows with branded educational modules, My. Oralspectrometry bridges the gap between experimental omics and accessible learning. The tool supports AI-trained histopath slide detectors and workflow synthesis, allowing students and clinicians to engage with spectrometric data in a practical, modular format. This work demonstrates how computational approaches can advance omics education and contribute to precision medicine by improving understanding of biomarker pathways and disease processes. The app is specially made for detection of various types of Oral Cancers and studying about its proteins and metabolites components and behaviour.

Keywords: Computational omics, proteomics, oral cancer, education
Theme: Computational Omics

SPEC/26- 041

Explainable Machine Learning Framework for SERS Identification of Bacterial Pathogens

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Rapid identification of bacterial pathogens is essential for timely treatment and infection control, but traditional culture-based methods take 24–48 hours, delaying care and worsening antimicrobial resistance (AMR). AMR poses a major public health threat, increasing deaths and healthcare costs, making fast, accurate diagnostics vital for guiding proper antibiotic use and improving patient outcomes.

Surface-Enhanced Raman Spectroscopy (SERS) offers a promising label-free, rapid diagnostic alternative by capturing unique molecular fingerprints of bacterial cells, enabling the detection and identification of pathogens within a much shorter timeframe compared to conventional methods. This study combines SERS with advanced machine learning (ML) algorithms and SHAP (SHapley Additive exPlanations) analysis for explainable discrimination of clinically relevant bacterial pathogens.

Five clinically important bacterial species were investigated: Enterococcus faecalis, Pseudomonas aeruginosa, methicillin-resistant Staphylococcus aureus (MRSA), Staphylococcus aureus, and Klebsiella pneumoniae. Among the tested models, Support Vector Machine (SVM), k-Nearest Neighbour (kNN), Random Forest (RF), and a 1D Convolutional Neural Network (CNN), the CNN achieved near-perfect classification accuracy, capturing subtle vibrational variations often inaccessible to traditional algorithms.

To ensure transparent decision-making, SHapley Additive exPlanations (SHAP) analysis was applied to both RF and CNN models. Remarkably, both frameworks converged on the same discriminatory Raman regions revealing conserved biochemical determinants of species identity. Complementary MCR-ALS decomposition further resolved the spectra into interpretable biochemical components. Together, this study aims to demonstrate an end-to-end explainable SERS workflow that couples SERS with interpretable AI, offering a rapid, transparent approach for pathogen diagnostics and AMR surveillance.

This interpretability is crucial for clinical adoption, as it enables transparent decision-making and fosters trust in AI-driven diagnostics. The application of AI in healthcare, particularly in pathogen detection and AMR management, is revolutionizing clinical microbiology by enabling faster, more accurate, and scalable diagnostic solutions.

SPEC/26- 042

Cancer Energetics: Integrated Consumption-Release and Pool Size Mapping Reveals Convergent and Divergent Metabolic Signatures Across Glioma, Melanoma, and Colorectal Cancer Cells

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Metabolic reprogramming enables cancer cells to sustain proliferation under diverse stresses by redirecting carbon and nitrogen fluxes. To characterize this metabolic plasticity, we integrated extracellular consumption-release (CoRe)fluxes with intracellular metabolite pool quantification using ^{1}H-NMR spectroscopy across glioma, melanoma, and colorectal carcinoma cells. Glioma cells showed high glutamine and threonine uptake with moderate lactate secretion, indicating a balanced oxidative-glycolytic state, whereas melanoma and colorectal carcinoma exhibited stronger glycolytic and glutaminolytic activity. Melanoma uniquely released acetate and succinate, suggestive of truncated TCA cycling, while colorectal carcinoma displayed enhanced alanine transamination and osmolyte turnover. Principal component clustering revealed two dominant axes: glucose-lactate and glutamine-glutamate coupling, transcending tissue origin. These findings highlight that metabolic phenotype, rather than lineage, defines tumour bioenergetics and demonstrate a scalable, non-invasive NMR-based platform for metabolic phenotyping with translational potential for in vivo applications.

SPEC/26- 043

Potential-Modulated SERS Profiling via GLAD-Fabricated Ag Nanorod Arrays for Ultrasensitive and Label-Free Spectro-electrochemical Sensing

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Routine analysis of food adulterants and pharmaceutical additives at the point of care is crucial for food safety and environmental protection. Surface-enhanced Raman spectroscopy (SERS)-based sensing has gained significant importance in various scientific and technological domains, including analytical chemistry, biomedical diagnostics, forensic science, drug discovery, environmental monitoring, and food safety. Electrochemical SERS (EC-SERS) enhances the technique by regulating surface charge, adsorption, desorption dynamics, and redox processes, improving signal intensity and selectivity. Despite having advantages, developing EC-SERS sensors for field applications remains constrained by the limited availability of robust and reproducible SERS-active electrochemical substrates. This study introduces a cutting-edge portable EC-SERS platform, leveraging silver (Ag) nanorods engineered onto screen-printed electrodes via a thermal evaporation-based glancing angle deposition (GLAD) technique. This innovative approach ensures exceptional signal enhancement, outstanding sensitivity, and remarkable reproducibility, making it a powerful tool for high-precision molecular detection. Potential-modulated SERS profiling of p-aminothiophenol, 1,2-bis-(4-pyridyl)ethylene, and melamine was carried out at various electrochemical potentials. Additionally, the maximum signal enhancement was achieved at an optimized potential (Vmax), enabling the detection of melamine with a remarkable limit of 10 pM, surpassing previously reported substrates. The results highlight the promise of GLAD- fabricated AgNRs@SPE as a sensitive, label-free, reusable, and portable EC-SERS platform. This platform will present significant improvements in detecting analytes relevant to analytical chemistry, the pharmaceutical industry, and drug control.

Keywords: p-aminothiophenol, screen-printed electrodes, electrochemical SERS, glancing angle deposition.

SPECTROMICS - 2026

SPECTROMETRY-INTEGRATED OMICS IN HEALTH AND DISEASE

16th –17th January

Inspiring Ideas, Capturing Imagination

INNOVATION GALLERY

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ABOUT IIT DHARWAD

Academic Excellence

IIT Dharwad is one of the third-generation IITs established in 2016 by the Ministry of Education, Government of India. The institute is committed to excellence in teaching, research, and innovation across diverse disciplines of science and engineering.

With a vibrant and growing campus spread across a 470-acre permanent site, IIT Dharwad offers a dynamic academic environment supported by state-of-the-art laboratories, advanced research facilities, and a collaborative culture. The institute fosters interdisciplinary learning and emphasizes both foundational knowledge and emerging technologies to address real-world challenges and is steadily growing into a hub of academic and research excellence.

📍 Location & Heritage

IIT Dharwad is located on the outskirts of Dharwad, which is part of the twin cities of Hubballi-Dharwad in the north of Karnataka. Known for its pleasant climate year-round 🌤️, Dharwad is a picturesque locale positioned between the Western Ghats (Malenadu) ⛰️ and the Deccan Plains (Bayalu Seeme).

Dharwad derives its name from the Sanskrit word "DWARAWATA" 📜. The twin cities are famous for their rich culture, literature 📚, and pivotal role in the Indian freedom movement 🇮🇳. It is an academic hub 🎓, home to institutions such as IIIT Dharwad, University of Agricultural Sciences, Karnataka University, and the National Forensic Sciences University.

Exploring the Region 🗺️

Beyond the campus, the region offers a blend of history and nature:

Kittur Fort (20 km): 🏰 Historic site where Rani Chennamma fought the British in 1824.

Dandeli National Park (60 km): 🐆 Ideal for wildlife enthusiasts and adventure seekers.

Goa (150 km): 🏖️ Famous for its beaches and Portuguese heritage.

Hampi (190 km): 🏛️ A UNESCO World Heritage site featuring the ruins of the Vijayanagara Empire.

Dudhsagar & Jog Waterfalls (190 km): 🌊 Spectacular natural waterfalls.

Belur & Halebidu (350 km): 🛕 Renowned for intricate Hoysala architecture.

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