

Mini symposium on Metabolomics and Volatomics towards disease markers



May 16, 2016

Convener: **Dr. Srikanth Rapole, Scientist,**
Proteomics Lab, NCCS, Pune.



The mini symposium on "**Metabolomics and Volatomics towards disease markers**" was organized at National Centre for Cell Science, Pune on 16th May 2016. This event was funded by New INDIGO program of the Department of Biotechnology.



The symposium was formally inaugurated by **Dr. Shekhar Mande**, Director NCCS. It was followed by a welcome address by **Dr. Surekha Zingde**, President, Proteomics



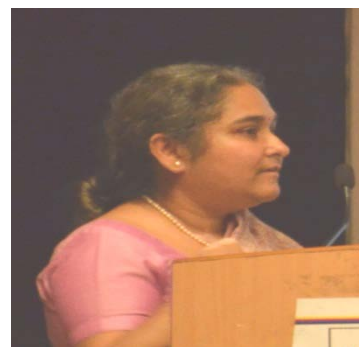
Society, India. She highlighted the necessity of having lecture workshop on Metabolomics and Volatomics, where the current status in the field could be shared with the new researchers and they get an opportunity to meet and discuss with experts in the field.



On behalf of NCCS Pune and the organizers **Dr. Srikanth Rapole**, convener of the mini symposium, welcomed the eminent speakers, authorities and the delegates of the symposium and briefed the importance of Metabolomics and Volatomics field and idea behind organizing this event. He explained that the symposium was arranged to highlight the concept and scope of metabolomics to the students and faculty from research and academic institutions. He discussed about the advances in mass spectrometry technology and how it enabled researchers to identify thousands of metabolites with high accuracy in a single experiment. Metabolomics and Volatomics approach enables the discovery of metabolic signatures for various diseases using non-invasive sampling methodologies.

This was followed by 14 lectures arranged in four sessions.

Session I -“Metabolomics Towards Biological Mechanisms & Biomarkers” was chaired by **Dr. Surekha Zingde & Dr. Anjali Shiras**.



The opening talk by **Dr. Harsha Gowda**, from Institute of Bioinformatics, Bangalore entitled ‘Untargeted and targeted metabolomics to identify biomarkers and understand disease mechanisms’ was very impressive as he discussed how the advent of mass spectrometry based metabolomics has enabled identification and quantitation of metabolites in a high-throughput manner and these studies can be carried out by employing both targeted and untargeted approaches which are useful to understand disease mechanisms and identify biomarkers.

The second talk ‘Identifying metabolite markers for coronary artery disease using an untargeted metabolomics approach’ by **Dr. Shantanu Sengupta**, Institute of Genomics and Integrative Biology, New Delhi, was highly informative where the early detection of

coronary artery disease (CAD), the largest cause of mortality and morbidity in developing countries using an untargeted metabolomics approach was discussed. Using the untargeted metabolomic approach 32 candidate metabolites were identified that show altered levels in CAD patient's plasma and carry a potential as disease marker.

The third talk 'Understanding proteo-metabolomic networks modulating nutrient response and immunity in plant' was delivered by plant proteomic expert **Dr. Subhra Chakraborty**, National Institute of Plant Genome Research, New Delhi. Her work elaborated on how the proteo-metabolomic approach was used to determine the cellular circuitry that operates in plant immunity during fungal disease. Oxalic acid, a small molecular weight metabolite, was recognized as a food toxin which plays dual role in fungal pathogenicity in a concentration dependent manner. The role of acid homeostasis and the translational and metabolic reprogramming during non-host resistance was revealed.

Session II: "Metabolomics Of Infectious Diseases" was chaired by **Dr. Musti V. Krishnasastri & Dr. Shantanu Sengupta**.



First talk of the second session 'Transcriptomic, proteomic and metabolomic analysis of sexual stage development in Malaria' by **Dr. Utpal Tatu**, Indian Institute of Science, Bangalore was highly educative; explaining how the malarial parasite responds to stress during its growth. Global profiling of gene expression, proteomic and metabolomic profiling together revealed a network of transcription factors, their targets and specific metabolites being activated and/or upregulated upon redox stress. The study was useful in understanding the intricate biology of parasite life cycle.

Next, **Dr. Sanjeeva Srivastava**, Indian Institute of Technology Bombay, Mumbai presented his work entitled, 'Comparative proteomic and metabolomics analysis of

severe and non-severe cohorts of Malaria patients for identification of potential prognostic serum biomarkers and understanding pathobiology of disease.’ He explained how serum samples from patients across different endemic regions of India were examined using quantitative proteomics platforms like DIGE and iTRAQ and a metabolomics approach using LC-MS to identify markers of disease severity.

Third presentation was by **Dr. Sharmistha Banerjee** on ‘Understanding mycobacterial pathogenesis and Mycobacteria-HIV coalition through comparative proteomics and metabolomics’ from School of Life Sciences, University of Hyderabad, Hyderabad. Dr. Sharmistha presented her work with focus on proteomic and metabolomics analysis in deciphering the coalition between two major human pathogens: Mycobacterium tuberculosis (the tuberculosis causing bacteria) and HIV. She elaborated on the use of proteomics to understand the molecular events involved and identify differentially regulated proteins during mycobacteria-HIV co-infection.

Fourth presentation in second session entitled ‘Metabolic phenotyping of pulmonary tuberculosis patients at diagnosis and during treatment’ was delivered by **Dr. Ranjan Nanda**, Translational Health Group, International Center for Genetic Engineering and Biotechnology, New Delhi. He explained how infection induced metabolic alterations may reflect in host biofluid metabolic phenotypes. Differential analyses of deregulated urine metabolites and exhaled breath volatile organic compounds of Active-TB and Non-TB subjects at diagnosis and during therapeutic intervention were discussed. Long term goal of his work is to develop an easy to use point of care TB screening tools in eNOSE format and to identify important host metabolites that could be useful as candidates for TB adjunct therapy.

Session III: “Metabolomics Of Diabetes & Other Diseases” was chaired by Dr. Subhra Chakraborty & Dr. Mohana Krishna Reddy.

In third session, **Dr. R. Srinivas**, senior faculty from Indian Institute of Chemical Technology (IICT), Hyderabad, presented his work entitled ‘HR LC/MS study on vitamin D metabolites in coronary artery disease and type 2 diabetes in south Indian patients’. His work revealed that lower vitamin D levels were linked with metabolic diseases like type 1 diabetes, obesity, insulin resistance, cardiovascular diseases, and

cancer. Patient sample analyses carried out using LC/APCI/HRMS approach to determine levels of six vitamin D metabolites revealed association of vitamin D and metabolites with type 2 diabetes and coronary artery disease.



Second talk in third session entitled ‘ESI-MS/MS studies on methylated and AGE products of metabolites: Candidate biomarkers of diabetes’ was delivered by **Dr. S. Prabhakar**, Indian Institute of Chemical Technology, Hyderabad. He described use of the mass spectrometry techniques to study Advanced Glycation End (AGEs) products of metabolites at protein/DNA level. Analyses of methylated metabolites, characterization of all possible mono, dimethylated amino acids and betaines for generation of biomarker were the highlights of the talk. He also stated the future plan for generation of database for methylated molecules.

Next was a very intriguing talk entitled ‘NMR based metabolomics: Biomarker discovery and understanding of disease pathology’ by **Dr. Koel Chaudhury**, Indian Institute of Technology Kharagpur, Kharagpur. She elucidated the current status in metabolomic investigations involves two complementary tools - NMR and chromatographic separation (gas chromatography or liquid chromatography) followed by mass spectrometry. Mass spectrometry was more sensitive and NMR was more robust and reproducible, and can be used to analyze intact biofluids with little or no sample preparation. She explained that Carr Purcell Meiboom Gill (CPMG) pulse sequence was used for suppression of resonances from high-molecular weight species, facilitating the observation of low molecular weight metabolites ($\leq 1500\text{kDa}$) and how this was utilized towards understanding of pathophysiology and biomarkers identification of various women’s health related disorders.

The last talk in third session was delivered by **Dr. Soumen Kanti Manna** from Saha Institute of Nuclear Physics, Kolkata. His talk entitled ‘Metabolomics: Expanding the

Horizon' elaborated on how targeted and untargeted metabolic profiling contributes in identifying potential biomarkers for exposure, diseases and disorders. Advances in chromatography and mass spectrometry have enabled an ever richer view of the biochemical landscape largely unexplored so far. He talked about application of metabolomics in liver diseases, colorectal cancer, lung cancer and breast cancer and how unprejudiced knowledge of chemistry can help in unraveling novel metabolites and metabolic pathways.

Session IV: "Metabolomics & Volatomics Towards Disease Markers" was chaired by **Dr. R. Srinivas & Dr. Sanjeeva Srivastava.**



The first presentation of fourth session entitled 'Investigation of metabolomic, lipidomic and volatomic alterations towards potential biomarkers in Breast Cancer' by **Dr. Srikanth Rapole**, National Centre for Cell Science, Pune. His work encompassed comparative analyses of the metabolome in Breast cancer study. He talked about comparative analyses of normal, benign and malignant serum, urine and tissue samples for a better understanding of the molecular events in tumor development. Analysis of serum and tissue samples was done using LC-MS and GC-MS platforms. For phospholipid profiling, lipids were analysed by in house MRM based approach using AB Sciex 4000 QTRAP LC-MS/MS. He also talked about the development of urinary metabolomic biosignatures of breast cancer patients and healthy individuals (control group) and to explore the VOMs as potential biomarkers in breast cancer diagnosis at an early stage.

'Potential of saliva volatomics for the non-invasive profiling and discrimination of cancer - preliminary studies with breast and lung cancers' by **Dr. Jorge A. M. Pereira**,

University of Madeira, Portugal was second presentation in fourth session. He talked about saliva volatomics having a remarkable potential for the non-invasive characterization of cancer development. His work involved use of dynamic headspace solid phase micro extraction (HS-SPME) followed by Gas Chromatography coupled to Mass Spectrometry (GC-MS) for screening of saliva samples from breast and lung cancer patients.

The last talk of the day entitled 'Breath analysis: A promise to non-invasive clinical diagnosis?' by **Pritam Sukul**, Rostock University Medical Center, Germany. He presented data of how different breathing patterns are obtained with changes in postures and forced respiratory manoeuvres in spontaneously breathing healthy human subjects to induce physiological effects onto the composition of exhaled breath. He also talked about how advanced real-time mass-spectrometric techniques such as SIFT-MS, and different PTR-MS in association with online end-tidal (alveolar) sampling have significantly lowered many confounding factors like environmental, dietary intake or bacterial emission and clinical contaminations that are contributing to VOC patterns equally as pathophysiological conditions or biological processes.

Overall, all the scientific talks of symposium were highly informative and motivating for the participants. Young scientists **Dr. Amol Suryawanshi** from Institute of Life Sciences, **Dr. Jagadeshwar Reddy** from Central Drug Research Institute, **Dr. Mohana Krishna Reddy** from Indian Institute of Chemical Technology also actively participated. The event was formally concluded by vote of thanks from **Dr. Jyoti Rao**, Scientist, NCCS.

