NEWS

Second international symposium on mass spectrometry in life sciences

Bangalore, India, August 23–26, 2011

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Over 100 delegates attended the 2nd International Symposium on Mass Spectrometry in Life Sciences in Bangalore (http://www.ncbs.res.in/node/497). The symposium was organized by Dominik Schwudke and Sarita Hebbar from the National Centre for Biological Sciences (NCBS), which is part of the Tata Institute of Fundamental Research. After completing his PhD at Max Planck Institute of Molecular Cell Biology and Genetics in Dresden under the supervision of Prof. Andrej Shevchenko, Dr. Schwudke moved to Bangalore about two years ago to lead the biological mass spectrometry laboratory at NCBS, with the main research focus on lipidomics.

With an elevation of about 1000 meters and its location in the southern part of India, equally distant from East and West to the Indian Ocean, Bangalore has a welcoming moderate climate most of the year. The city is a major cultural and economic hub in India, also known as Silicon Valley of India due to its strong IT industry. Several global analytical, biotech and pharmaceutical companies have set up their R&D laboratories in Bangalore. NCSB has been setting up several excellent facilities for biological research, including the mass spectrometry facility (Fig. 1).

The symposium programme included two tutorial, 27 lectures and 6 poster presentations across the domains of proteomics, lipidomics and metabolomics. The symposium started on Tuesday 23rd August in the evening with an opening keynote lecture by Michael W. Linscheid from Department of Chemistry at Humboldt University Berlin, with the title "Of music, math and measurement". This inspiring talk provided a fresh perspective on the nature of

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measurement, with emphasis on spectroscopic methods to measure biomolecules, by comparing such studies to generation of and listening to the music. As one example of alternative use of NMR instrument, although unlikely to impress the funding agencies, Dr. Linscheid mentioned how NMR can be used for generating music (http://www. chemie.uni-erlangen.de/bauer/music.html). Following the lecture, the participants were welcomed by the outdoor reception and dinner at the NCBS lawns as well as by a concert by the Ananth Menon Quartet.

On Wednesday morning the programme started with a tutorial on mass spectrometry in "omics" research, given by Dominik Schwudke. The tutorial was followed by a session on proteomics and in the afternoon by a session on lipidomics. In the latter, Stephen J. Blanksby from University of Wollogong, Australia, discussed recent advances in complete structural elucidation of complex lipids by using ozone induced dissociation (OzID) and radical directed dissociation (RDD). These methods can differentiate double bond- and stereo-isomers and therefore hold promise to greatly improve our ability to identify the presence of lipid diversity. However, several challenges still remain, including the sensitivity of the methods as well as ability to implement them in typical highthroughput experimental lipidomics setting, which will likely require further instrumental advances. In principle, the OzID and RDD method may also be applicable to structurally elucidate other small molecules than lipids.

Andrej Shevchenko's lecture presented the methodological considerations when implementing a lipidomics platform for biological research. Recent advances, particularly in shotgun lipidomics, have provided analytical and software tools for setting up lipidomics as a routine method in the research laboratory, enabling rapid, accurate and quantitative characterization of molecular lipid species. Markus Wenk from National University of Singapore described a

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Fig. 1 National Centre for Biological Sciences (NCBS) in Bangalore (entrance shown in *left*) has established several core facilities for biological research. These include molecular imaging, transgenic fly and mouse genetics facilities, with the latter being set up in

collaboration with the RIKEN institute from Japan. Recently, mass spectrometry facility was established (*right*) under direction of Dr. Dominik Schwudke

lipidomic study of meibum samples from patients with dry eye syndrome and control subjects. Comprehensive lipidomic analysis included quantification of (O-acyl)-omegahydroxy-fatty acids (OAHFA), which were also found consistently decreased in patients, with their levels decreasing with increasing disease severity. Dominik Schwudke presented a multi-omic approach performed at NCSI to study neurodegeneration and aging in Drosophila melanogaster. Quantitative lipidomics was performed along with imaging and behavioral assays to functionally characterize the roles of sphingolipids in the process of neurodegeneration and calcium signaling in the control of neutral lipid homeostasis. Matej Orešič presented recently published research that led to understanding of how adipocyte lipid membranes adapt to obesity, and how this adaptation may lead to higher vulnerability of adipose tissue to inflammation and therefore to metabolic disease. As part of this study a novel computational approach was introduced to help interpret the cellular lipidomes. Lipid bilayers were reconstituted based on lipidomics data using the computationally intensive atomic scale molecular dynamics simulations.

On Thursday morning the programme started with a tutorial on soft ionization method by Klaus Dreisewerd from University of Münster, Germany. This was followed by a session on proteomics and in the afternoon by a session on analysis of metabolites and small molecules. The metabolomics session focused on analytical advances to detect and profile small molecules in biological samples, with the emphasis on molecular imaging and in vivo analysis. For example, Venkateswarlu Panchagnula from National Chemical Laboratory (Pune, India) described developments of a robust platform for high-throughput profiling of trace metabolites using laser desorption/ionization mass

spectrometry (LDI-MS). The results using this platform were found comparable to conventional LC-ESI-MS platform, with an added advantage of faster analysis. Joanne Y. Yew from National University of Singapore described how an application of metabolomics in vivo led to discovery of novel pheromones in Drosophila. UV-LDI-MS and direct analysis in real time (DART)-MS was applied to study the lipid composition of cuticular extracts or intact flies (D. mojavensis and D. arizonae), followed-up by behavioral experiments and detailed structural characterization of lipids by using HPLC-ESI-MS/MS and GC-MS. The UV-LDI-MS and DART-MS analyses identified a putative novel class of sex-specific triglycerides with short fatty acyl chains and long-chain hydrocarbons expressed on the cuticular surface of Drosophila. Behavioral experiments showed that these lipids likely play a role as pheromones that influence the mating choice.

The poster sessions on Wednesday and Thursday included 45 contributions, mainly from Indian metabolomics and proteomics laboratories. These sessions demonstrated that there has been a great deal of investment and interest in proteomics and metabolomics over the past years in India, and much can be expected in the coming years from researchers in India in these domains.

The symposium organizers would like to thank to all the supporters and sponsors including Department of Biotechnology of Government of India, The Wellcome Trust/DBT India Alliance, Agilent Technologies India Pvt. Ltd., Waters India Pvt. Ltd., AB Sciex and Labindia, and Thermo Fischer Scientific India Pvt. Ltd. Many congratulations should go to organizing committee for the scientifically and socially interesting symposium and to the attendees who presented their interesting scientific research.