OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference and Exhibition on
Analytical & Bioanalytical Techniques
November 22-24, 2012   Hyderabad International Convention Centre, India

High resolution mass spectrometric approaches for the comparative profiling of bioactive components of leaf extracts of tulsi varieties

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The recent advancements in the instrumentation and techniques have made mass spectrometry, the most sensitive and widely used analytical method. Such advancements have opened up the possibilities of identification and structural analysis of bioactive compounds present in low quantities which were difficult to detect with the conventional approaches. This presentation will give an overview of the targeted and non-targeted workflows utilizing power of high resolution accurate mass spectrometry for comparative screening of phytochemicals among various plant species. The analysis of these bioactive compounds is essential to understand the secret of their effectiveness.

Three varieties of Tulsi (*Ocimum*) viz Rama (*Ocimum sanctum*), Krishna (*Ocimum sanctum*) and Vana (*Ocimum gratissimum*) were screened using a generic High Resolution Mass Spectrometric (HRMS) workflow followed by Principal component analysis (PCA) to identify the relative variations of the common phytochemicals present in the plant. Simultaneous TOF MS and MS/MS allowed accurate mass of parent ions and MS/MS data to be used for analyte identification and confirmation on a single injection. Preliminary statistical analysis by Principal Component Analysis (PCA) and t-Test processing using MarkerView™ software differentiates three varieties and the bioactive components contributing to the differences between the species. Targeted analysis using XIC manager was carried out using the m/z of 94 compounds reported in literature associated with *Ocimum*. Subppm mass accuracy which is a prerequisite for alignment and profiling of complex extracts has been obtained in all the TOFMS and TOFMS/MS analysis. Formulae prediction using the high resolution MS/MS fragmentation data with Formula Finder tool within PeakView™ Software was used to predict the best possible elemental composition and ultimately compound identification. We have been able to identify several compounds that differentiated the three different varieties of Tulsi. Thus, the present study shows that high throughput identification and comparison of bioactive compounds in different plant species can be achieved by using high resolution mass spectrometric analysis.

Biography

Annu Uppal completed her PhD in Biotechnology from The Indian Institute of Toxicology Research, Lucknow and did her Postdoctoral fellow at School of Life Sciences, Jawaharlal Nehru University. She has more than twenty-nine research papers and book chapters published in peer reviewed journals. She has an extensive experience in giving presentations in International & national conferences. Currently she is with AB SCIEX as Application Support Scientist, and is responsible for support and application development in the proteomics, metabolomics, lipidomics and bioanalysis using high resolution mass spectrometry

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J Anal Bioanal Techniques 2012
ISSN: 2155-9872, JABT an open access journal

Analytica Acta-2012
November 22-24, 2012

Volume 3 Issue 7
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