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Dereplication and optimization through intact cell mass spectrometry for non-ribosomal peptide producers from natural products

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Natural products are an unfurled promising resource with magnanimous diversity. With millions of years of continuous evolutionary development natural resources viz. microbes have acquired incredible adaptability due to their strong flexible metabolic power as potential resources of new drug leads. The wonderful interaction of molecular dialogue between the two organisms viz. microbe and plant induces dramatic changes and studies have shown that vast repertoire of genes are involved in this biosynthesis of secondary metabolites such as Non Ribosomal Peptides (NRPs), polyketides, terpenoids and pyrones. History witnessed major backtrack in drug discovery efforts from unfurled golden mine of natural products despite possessing magnanimous diversity due to frequent re-discovery of known compounds, trace level production, lengthy processing time and complex natural mixtures as some major challenges faced. Dereplication is therefore an exigent need at incipient stages of discovery processes. An expeditious and efficient dereplication strategy was applied on epiphytes and endophytes of medicinal plants, soil microbes using Intact Cell Mass Spectrometry [ICMS] technique. ICMS is a simple, rapid and sensitive technique for direct detection of peptaibiotics using MALDI TOF/TOF mass spectrometer. With microgram amount of sample and any prerequisite for chromatographic separations and processing, accurate reproducible results can be obtained giving quick insight into possible peptaibiotics producers. Study of optimization experiments at miniaturized level for maximized production of desirable secondary metabolites can also be carried out using this technique which saves time and resources and expedite drug discovery efforts from natural products.

Biography

Deepika Singh is Senior Scientist at Quality Control and Quality Assurance Division, CSIR-IIIM Jammu. She did her post graduation in Organic Chemistry and in Modern Methods of Chemical Analysis from IIT-Delhi. She has published more than 20 research articles. Her research interest lies in dereplication for identification of novel metabolites from natural products and their isolation and characterization. She has good experience and expertise in method development and validation of pesticides, heavy metals, antibiotic drug residues, vitamins and aflatoxins in agricultural and processed foods as well as in Chemistry Manufacturing and Control (CMC) of herbal extracts and formulations using modern analytical instruments like MALDI-TOF/TOF, LC-MS/MS, NMR, HPLC, GC-MS/MS and ICPMS.

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