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LC-MS/MS based dereplication tool in identification of plant secondary metabolite

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Identification of compounds from natural sources, like plant extract etc, has resulted in discovery various pharmacologically active agents. Since, isolation of lead compounds is incredibly time-consuming, the efficient and reliable identification of compounds in plant extracts isolated previously is essential. Thus, dereplication becomes an important process before proceeding bioassay-guided isolation. Mass spectral data are important in identification of chemical constituents. LC-MS/MS has been a tool to chromatographically isolate the chemical constituents and mass spectrometer record the mass fragmentation profile. This fragmentation pattern, offers a unique molecular signature of organic compounds. The characterization of the mass fragments to identify the constituent requires comparison with the standard spectra. Most the published mass spectral data are of limited information. The spectral data publish are often difficult to compare manually with the data obtained by other researchers.

We developed a open source LC-MS/MS data repository of natural product compounds (www.tmsdatabase.org). The data base can be accessed by user worldwide and use software algorithm for structural identification of unknown molecules. The web based search engine www.tmsdatabase.org has a built-in software feature for spectral repository, spectra retrieval and spectral comparison. The mass fragments data of various experimental conditions in different instruments are consolidated as single compound database. The user can view the mass spectra with detail experimental condition/instrument in the web based interface. In case of unknown the mass spectra the user can upload mass data for compound identification. Algorithms are built in software to identify the most feasible identity of the compound.

Biography

Rabi Sankar Bhatta is working as Scientist, Pharmacokinetic and Metabolism Div., in Central Drug Research Institute, an new drug discovery research institute. He has ten years of experience in various academic and pharmaceutical industrial experiences. His research interests include bioanalysis, metabolite identification, CYP profiling and pharmacokinetics of NCEs. He is actively involved in lead identification, preclinical and clinical development. He along with Dr. Sanjeev Kanojiya has developed web-based dereplication tool (www.tmsdatabase.org) for identification of plant secondary metabolite. He has guided several PhD, graguates students and has published several papers in reputed journals.