Digital Library of Indian Medicine Plants and their Metabolites: MS-based Bioinformatics Tool

(New Drug discovery & Exploration of Indian Medicinal Plants chemical diversity)

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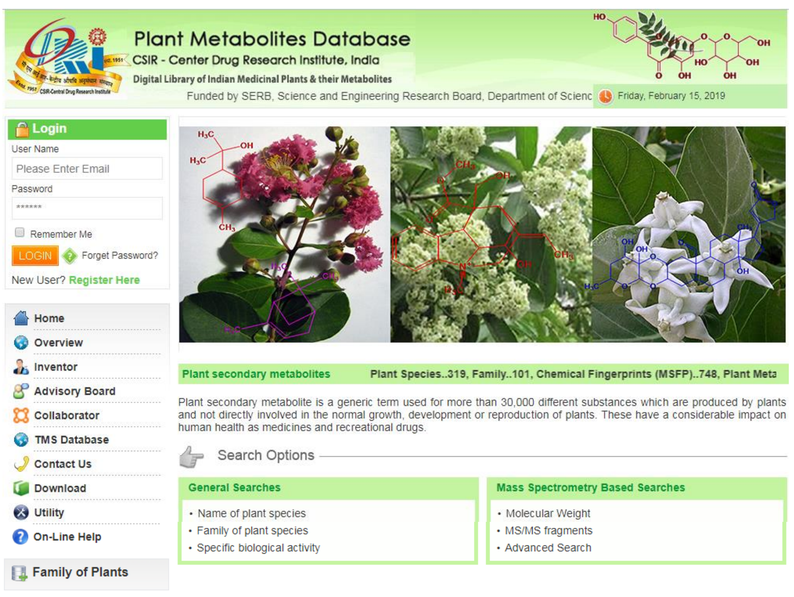
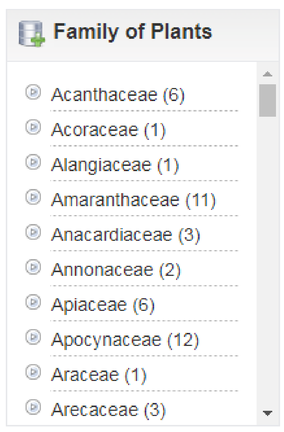
Overview

Over the past decades, high-performance liquid chromatography-mass spectrometry (LC-MS) has revolutionized analytical chemistry. The hyphenated MS techniques not only report the precise mass of compounds but also generate fragment ion spectra for identification/confirmation of compounds [1]. This fragmentation pattern offers a unique molecular signature of organic compounds. As a result, web-based LC-MS/MS library of plant secondary metabolites with suitable software search algorithm serves the purpose of inverse search (distribution of known bioactive compounds in different plant species). On the basis of above facts CSIR-CDRI, Lucknow developed a prototype of bioinformatics tool to explore chemical diversity of Indian medicinal plants.

Experimental: A universal reversed phase UPLC gradient program was developed for generation of UPLC/HPLC-MS profile (LC-MS fingerprint). The separation of wide range of plants metabolite were carried out on Waters BEH C-18 150 x 2.1 mm, 1.7µ column and developed MS/MS fingerprints of non-target plant metabolites. The HPLC, LC-MS and MS/MS fingerprints were utilized to develop the Digital Library of Indian Medicinal Plants & their Metabolites.

Results: A Web-based digital (LC-MS/MS) library of non-targeted plant secondary metabolites with suitable software search algorithm was developed (http://plantmetabolome.cdri.res.in) for exploration of Indian medicinal plants chemical diversity.



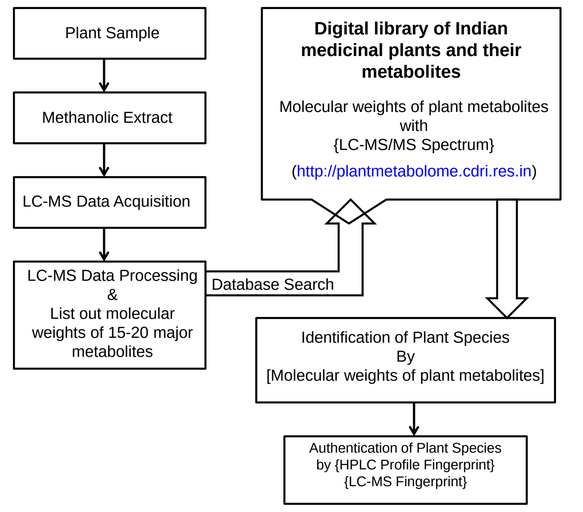


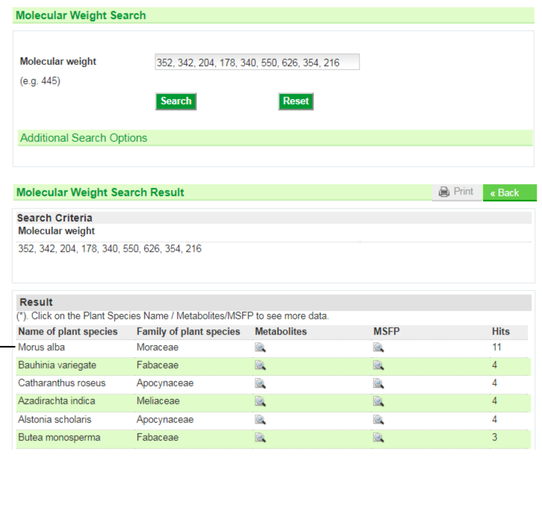
The above library provides mass spectrometry based methodologies to explore the chemistry of medicinal plants. It has targeted applications for natural product and medicinal plants chemistry.

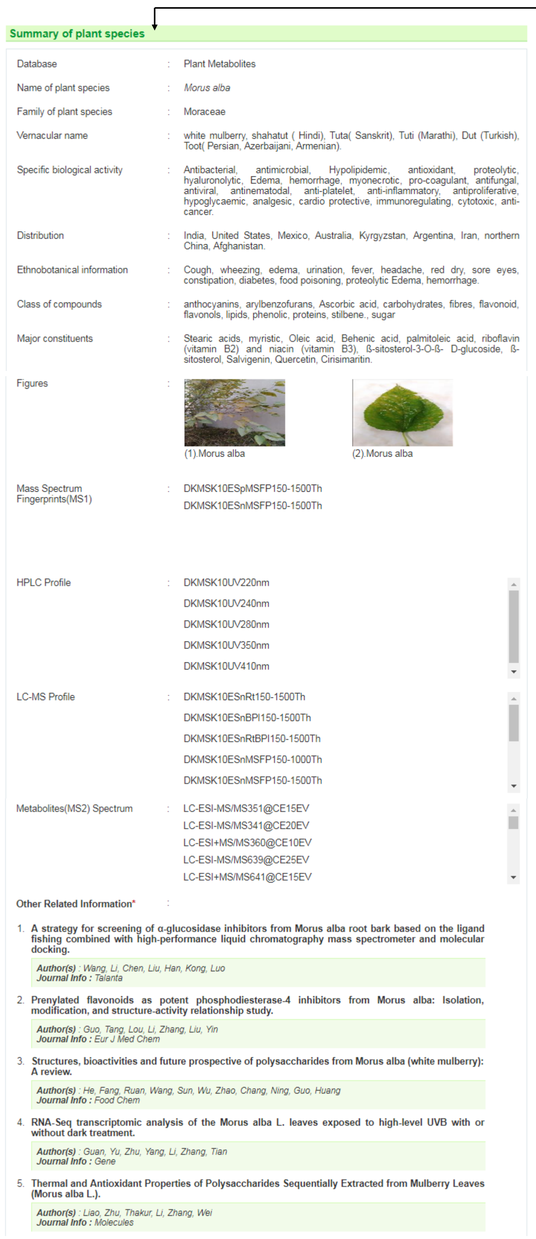
1. Identification and authentication of plant species based on their Mass Spectrum/HPLC/LC-MS Fingerprints.
2. Discovery of known bioactive compounds from previously unknown sources (*inverse search*).
3. Distribution of known compounds in different biological source (Plants/herbs).
4. Identification of known/unknown derivatives of bioactive compounds in different biological source (Plants/herbs) using LC-MS/MS data.

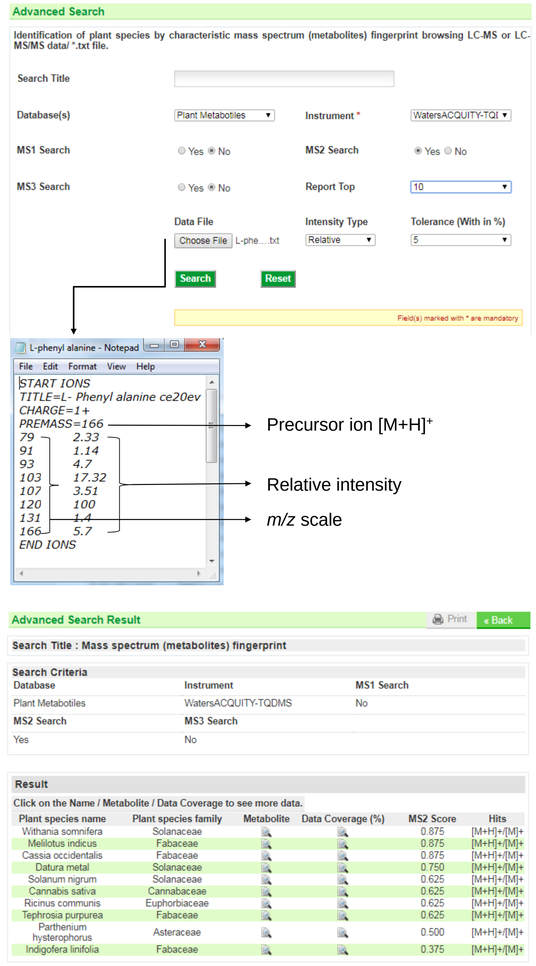
Currently, 319 medicinal plant species has been incorporated into Digital library from 101 families with more than 748 chemical/Mass spectrum fingerprints.

Mass spectrometry Based Search









- MS/MS based advance search results for identification of alternative natural source of L-phenyl alanine. *(L-phenylalanine is an essential amino acid and is the only form of phenylalanine found in proteins. Major dietary sources of L-phenylalanine include meat, fish, eggs, cheese and milk.)*
- MS2 Score: 1 = 100% Match, 0.80 = 80% Match, 0.72 = 72% Match
- Score > 60% is significant for identification of metabolite and it can be further validated by Retention time (Rt) of compounds in metabolite table.

Design and capabilities of tool/product: New research domain for exploration of natural products and chemistry of medicinal plants.

1. Worldwide contribution/accessibility/utilization of this library
2. Contribution in this library through data enrichment.
3. Knowledge sharing either on mutual understanding or payment basis.
4. Auto indexing of published scientific information on medicinal plants and natural products.

References:

1. Bouslimani, A.; Sanchez, L. M.; Garg, N.; Dorrestein, P. C., Mass spectrometry of natural products: current, emerging and future technologies. *Natural Product Reports* **2014,** 31, (6), 718-729.

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