Metabolomics and system biology: Next-generation medical diagnostics The advancement of metabolomics, which is the study of biological fluids in order to diagnose diseases, has allowed us to begin painting pictures of what is happening inside a cell or tissue. In particular, nuclear magnetic resonance is a promising method to analyze metabolites on a large scale, and has proven its success in the diagnosis of diabetes mellitus. Progress in this area has been limited by the difficulties associated with analyzing large datasets and spectral identity: due to the complex soup of chemicals that exist at any one point in time in a cell, the resultant overlapping “fingerprints” that identify a compound can be difficult to separate and identify accurately. As a result, NMR spectral identification and assignment remains extremely time and labor-intensive.

High-throughput assignment of NMR spectra for metabolomics MetaboID is a Matlab-based, open-source graphical user interface that can guide one-dimensional NMR spectral assignment. It draws its chemical shift lists and full resolution spectra for 360 unique compounds from publicly available databases, and also has 25 additional compounds whose data is collected in-house. MetaboID is built to guide assignment in order of increasing confidence. Assignment begins with library searches based on selected signals, followed by successive elimination and potential candidate compounds through NMR spectral comparisons. Refinement is performed by loading a full resolution NMR spectrum. The goal of this package is to provide high-throughput assignment of NMR spectra for metabolomics while retaining user customizability and ease-of-use.

Applications • Drug discovery and development • Preventive screening and diagnostics • Animal health and breeding • Agriculture and nutrition Advantages • Intuitive user interface • Large spectral library of common metabolites • Open source code for user-specific application development • Fully customizable compound spectral library

Inventors

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