
Reference: 14054  Category: Data Analysis

Features and Benefits

- Compared to existing software, MetPP uses the peak lists deconvoluted from the instrument data as input and additionally renders peak filtering and merging, retention index matching, time course analysis and pattern recognition.
- MetPP can be used for large scale studies and out performs existing software in statistical measures.

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Technology

Comprehensive 2D gas chromatography time-of-flight mass spectrometry (GCxGC-TOF MS) system brings more accurate and rich information about compound retention times and mass spectrum than a 1D GC-MS system, representing a powerful technique for analysis of metabolites in complex biological systems. The GCxGC-TOF MS system generates a huge amount of high-dimensional data in metabolomics study that require efficient and accurate data analysis algorithms to uncover the biological information. Currently there is a lack of bioinformatics systems available for this data analysis.

MetPP was developed for analysis of metabolomics data acquired on a GCxGC-TOF MS system. It has a modular design including project management and multiple data analysis components. It uses the peak lists deconvoluted from the instrument data as its input and then renders peak filtering and merging, uses retention index filtering methods to detect and remove false-identified metabolites, performing peak list alignment, normalization, statistical significance tests, pattern recognition, and time course study to investigate the abundance of progression of each molecule.

Markets Addressed

The University of Louisville is seeking a business partner interested in developing and commercializing a computational platform entitled metabolomics profiling pipeline (MetPP) for analysis of metabolomics data acquired on a two-dimensional gas chromatography time-of-flight mass spectrometry (GCxGC-TOF MS) where large data samples can be analyzed to assess metabolite differences between sample groups for the purpose of disease biomarker discovery, drug development, or any other comparative analysis.

MetPP could provide options for users to filter data from the peak lists generated by ChromaTOF using the peak quality information provided by ChromaTOF. It could be used across many different spaces to analyze GC-MS or GCxGC-TOF MS data.

Technology Status

- IP Status: Registered Copyright
- Development Status: Functional Software developed and executable code transferable
- Fields of Use Available: Please Inquire