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SimMet: Informatics tool for automating LC-MS and MS/MS based large metabolomic data processing and analysis

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Recently, there has been rapid growth in innovations related to liquid chromatography-tandem mass spectrometry (LC-MS/MS) based metabolite profiling studies. However, the lack of high throughput software tools has been one of the bottle necks. A typical metabolomics data analysis pipeline may include multiple software tools for example, using of a data processing tool to generate peak lists, a database search tool for metabolite profiling, other tools to validate metabolites using MS/MS data pattern matching or *in silico* fragment matching, tools for performing statistical analysis for identifying differential metabolites and pathways analysis for the identified metabolites. We have investigated some of the challenges we commonly face while processing raw data and identifying metabolites accurately. In order to address the challenges, we have developed SimMet. We introduce data filters in the software protocol that can effectively remove significant number of peaks corresponding to noise based on shape of the LC-peaks and data from LC-MS runs of blanks, QCs, technical replicates of the biological samples. The application of these filters prior to subjecting the data into conventional statistical techniques such as ANOVA, t-test, PCA etc. may be desirable since data can be reduced without compromising the actual information. This will also enable speedy analysis of large data that are common in mass spectrometry based metabolomics work flows. The software work flow will be demonstrated based on a food metabolomics experiment with data acquired on an LC-compact Qq-TOF mass spectrometer (Bruker Daltonik) system.

Biography

Ningombam Sanjib Meitei has completed his PhD; he is the Chief Scientific Officer at Premier Biosoft, a leading bioinformatics company that provides software solutions for mass spectrometry based proteomics, glycomics, metabolomics, lipidomics and imaging data analysis. He has been leading the development of novel informatics tools namely; SimLipid, a LC-, MALDI- MS/MS data analysis tool for lipid identification by annotating product ions corresponding to lipid head-groups, fatty acyls, Charge Remote Fragment ions etc.; SimGlycan, the only high throughput glycan/glycopeptide identification tool that can also quantitate glycans using reporter ions intensity and MALDI Vision, a comprehensive mass spectrometry imaging data visualization and analysis tool.

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