

Normalization Procedure for Chemical Profiles in Biological or Medical Samples Detected by Mass Spectrometry

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Technology description

Market Summary

Metabolomic analyses are used in clinical diagnostics for a number of disorders including metabolic, hematologic, and endocrinological disorders. However there is currently no universal normalization protocol for use with liquid chromatography/mass spectrometry (LC/MS)-based metabolomics. Without normalization, the results from these analyses can vary significantly between different mass spectrometers and even the same mass spectrometer from week-to-week runs. In addition, liquid chromatography is performed on different columns and under diverse conditions, which leads to variable elution times and different spectral outcomes. Although normalization methods have been proposed, these analyses have no external standard, use log transformations that are unable to deal with features that contain a zero value, and are only suitable for lipid profiling within a specific range of mass-to-charge ratios (300-1600).

Technical Summary

Emory researchers have developed a normalization procedure for metabolomics that allows for multiple comparisons of chemical features from a large number of samples. Unlike other procedures, this method utilizes external and internal standards to account for and allow corrections for inter-instrument variability. In this way, test samples can be collected at different times and analyzed by different LC/MS machines but can be compared to each other. By normalizing the peaks of the multiple internal and external standards, this method corrects for different ionization efficiencies via normalization of the peaks from the multiple internal and external standards. This procedure also minimizes the variability that occurs from different elution times. Finally, unlike proposed methods, it can be used with smaller biomolecules that have a mass-to-charge ratio of 85-850 which includes nucleotides, amino acids, lipids, pyrroles, alcohols, and amines.

Application area

Normalization procedure that allows for the direct comparison of high-throughput liquid chromatography/mass spectrometry (LC/MS) metabolomic data gathered from different individuals at different times.

Advantages

Samples used can be collected at different times and/or analyzed by different mass spectrometers.
Cumulative datasets can be compiled and datasets can be compared to each other.
Useful for clinical diagnostics and research.

Institution

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