GSTP
Seminar Series

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Automated Filtering of NMR Spectra:
A New Tool for the Discovery of Metabolites
Associated with Type 2 Diabetes

Abstract:

Nuclear Magnetic Resonance (NMR) has emerged as an important analytical tool in the field of metabolomics. Virtually all of the current methods for statistical analysis of complex NMR spectra rely on a smoothing procedure (binning) to condense spectral complexity and correct for variability in peak location. We have found that the traditional binning methods can introduce experimental variability. In response to this, we developed Automated Filtering of NMR Spectra (AFNS). AFNS is a processing program that uses a rolling binning algorithm, multiple binwidths, and t-statistic based filtering as a means of identifying significant features in complex spectra. As an initial application of this program, we analyzed proton spectra of liver extracts from two strains of mice: the C57BL6/J (B6) and BTBR, in both genetically obese (ob/ob) and lean (+/+) conditions. Although lean mice from both strains are healthy, the BTBR ob/ob mice develop severe diabetes. In contrast, B6 ob/ob mice remain resistant to diabetes despite obesity. AFNS revealed that liver extracts from B6 +/+, BTBR +/+, B6 ob/ob and BTBR ob/ob mice have distinct molecular profiles that cluster in three distinct groups corresponding to healthy, diabetic, and diabetes resistant mice. AFNS was more effective in separating these groups than traditional analyses and was less susceptible to processing related variability. We are currently using the molecular profiles associated with each group in order to map traits that are associated with type 2 diabetes.