Application of Bayesian Inference for the Deconvolution of Nuclear Magnetic Resonance Spectra to Assess Metabolic Alterations and Type I Diabetes Susceptibility

Lee, Yewon (School: James Clemens High School)

Proton nuclear magnetic resonance (1H-NMR) spectroscopy is commonly used in metabolomics studies involving the quantitation of complex bio-fluids and mixtures to correlate metabolic changes to biological phenomena. Often, metabolites present in these bio-fluids display several peaks on the 1H-NMR spectra that overlap or are altered from the spectrum of the pure compound due to biological matrix effects and peak shifts caused by other confounding factors such as pH variability and present ions, leading to difficulties in the efficient deconvolution of resonances. In this study, Bayesian modeling achieved through a Markov chain Monte Carlo algorithm is utilized to provide a computational deconvolution approach and subsequently applied to the metabolic profiling of urine to evaluate non-invasive potential biomarkers and establish a metabolic signature from LEW.1WR1 rat models with genetic susceptibility to spontaneous Type 1 diabetes (T1D), a chronic autoimmune disorder affecting pancreatic beta cell function and loss of glycemic control. 23 metabolites involved with the glucose, creatinine, ketone bodies, and amino acid metabolisms and the TCA cycle were quantified through Bayesian analysis. Metabolic alterations across susceptibility factors and phases prior to T1D onset were identified in all six pathways of interest, including metabolites pyruvic acid, acetoacetic acid, and oxoglutaric acid. This work provides a premise for investigating the pathogenesis and metabolic abnormalities of T1D with an automated analysis that contribute to the acceleration of the deconvolution process for one dimensional 1H-NMR spectra in future studies and provide a non-invasive and cost-efficient predictive indicator for diabetic progression.

Awards Won:

Third Award of $1,000