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The advantages of mass accuracy and resolution in lipidomics and metabolomics – case studies using ultra-high resolution time of flight mass spectrometry with direct analysis and interfaced to separation techniques

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Abstract

High resolution mass spectrometry (HRMS) has become a preferred tool in comprehensive differential analysis for metabolomic profiling associated with disease states. In its many forms it is used in the direct analysis of samples (no chromatography) with great results for lipidomics. HRMS has also been used when interfaced to liquid chromatography, gas chromatography, and capillary electrophoresis. Here each of these techniques is applied to the investigation of differential metabolomic profiling associated with different disease states, physiological fluids, and analytical approaches. Plasma samples are investigated using direct infusion analysis to differentially profile lipids from diseased and control rats in the Zucker model. This is compared to GC and UHPLC analysis of the same when interfaced to the same high resolution mass spectrometer. Urine and serum samples from two forms of cancer are analyzed and the differences in the levels of metabolites which are up or down regulated with disease are discussed for hepatocarcinoma and prostrate cancer. The ability to leverage mass spectral data having resolving power of up to 100,000 and mass accuracies below 1 ppm is discussed in the context of potential biomarker identification and selective relative quantitation. The enhanced and more facile identification of metabolites is demonstrated using a novel approach to fragment ion creation known as MSc2 in LCMS. The utility of soft ionization in conjunction with EI spectral information is leveraged to confidently identify metabolites in GC analyses using high resolution mass spectrometry. Finally, the utility of time of flight as the accurate mass platform is discussed in general, and specifically when interfaced to high efficiency capillary electrophoresis where narrow peaks and the need for fragment ion information is significant. These advances in the technologies and approaches applied to metabolomic analyses create a new path for future investigations and a portfolio of analytical approaches to he metabolomic scientist.

Biography

Patrick has completed his Ph.D at Purdue University under the guidance of Prof. Graham Cooks. After more than 15 years in biological mass spectrometry and biomarker research, he is currently the Director of Marketed Technology at LECO, a manufacturer of high performance time of flight mass spectrometers. He has published more than 40 papers in reputed journals and presented more than 50 orals at global conferences.