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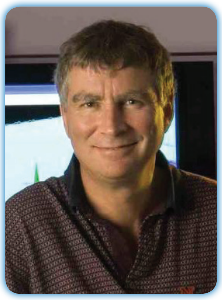

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Metabolomic analyses using comprehensive two-dimensional gas chromatography with mass spectrometry (GCxGC-MS)

Comprehensive two-dimensional chromatography, using either gas phase (GCxGC) or liquid phase (LCxLC) separation, is a powerful tool for complex chemical analyses such as are required for metabolomics. This paper presents results of preliminary GCxGC method development and data analysis for metabolomic investigations with *Arabidopsis thaliana*. The experiments analyzed three examples each of two types of Arabidopsis, Columbia (Col-0) ecotype and MutS HOMOLOG1 (MSH-1) T-DNA mutant. For each sample, three chromatographic replicates were performed using a Shimadzu GCMS-QP2010 Ultra gas chromatograph and single quadrupole mass spectrometer with Zoex ZX2 cooled-loop GCxGC thermal modulator, resulting in eighteen GCxGC-MS chromatograms. The chromatograms were visualized, processed, and analyzed with the GC image GCxGC software. The data processing generated a template pattern of peaks that could be reliably matched across chromatograms and those peaks were used to align and composite all eighteen chromatograms, and then built a feature template comprised of the reliable peaks and the 2D polygonal peak-region windows for all peaks detected in the composite chromatogram. The feature template was aligned to each chromatogram and the peak-region features used to generate a feature vector with mass spectrum for each region in each chromatogram. The feature vectors were analyzed using Fisher Linear Discriminant Analysis (LDA) to select highly discriminatory peak-regions with respect to class differences between the Col-0 and MSH-1 samples. The spectra of these regions were matched to several mass spectral libraries for preliminary identifications. Further analyses are being conducted with high-resolution mass spectrometry to indicate elemental compositions.

Biography

Stephen E Reichenbach is a Professor in the Computer Science and Engineering Department at the University of Nebraska - Lincoln. He earned his Ph.D. from the College of William and Mary and has held post-doctoral positions from the National Science Foundation, NASA, and the University of Manchester, Institute of Biotechnology. His research focuses on methods and tools for visualizing, processing, and analyzing multidimensional chemical data, especially from comprehensive multidimensional chromatography. He is the founding director of GC Image, LLC, a commercial spinoff of his research, which is a global leader in software for multidimensional chromatography.

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