

Differentiation of the plant materials using a Flow-Injection Mass Spectrometric (FIMS) fingerprinting method

Pei Chen

U.S. Department of Agriculture, USA

Producing a comprehensive overview of the chemical content of biologically-derived material is a major challenge. Methods used to profiling of such chemical content are usually long and laborious. Apart from ensuring adequate metabolome coverage, there are major technical difficulties associated with data pre-processing and signal identification. To address these factors flow-injection electrospray mass spectrometry (FIMS) has been developed as a high throughput metabolite fingerprinting tool. With little sample preparation, no chromatography, and instrument cycle times of less than 2 min, it saves significant resources (manpower, chemical reagents, column, and time) compared to other methods. Data pre-processing usually include aligning extracted mass spectra; generate mass-intensity matrices, and chemometric analysis.

The method has been applied to differentiating between skullcap from Germanders, between cinnamon species, between ginseng species, between of di and tetraploid *Gynostemma pentaphyllum* (Thunb.) Makino, between organically and conventionally grown grape fruits, peppermints, and sages. In addition to differentiating between the samples, the method can also pin point exactly what components in a sample set are responsible for the chemical difference detected. Combined with high-performance liquid chromatography (HPLC) and high-resolution accurate mass (HRAM) mass spectrometry (MS), the components that are responsible for the chemical differences can usually be annotated or identified. Not only can the method be used as a dietary assessment method, it can also be used to help design better, more meaningful and insightful nutritional or clinical studies.

pei.chen@ars.usda.gov