

Title: Aroma Profiling of Coffee with GC, GC×GC, and TOF MS

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Abstract

Coffee is one of the most consumed beverages in the world and the industry around it is an important part of the global economy. As expected with commodities, there is a large amount of taste and flavor variation in coffee that can relate to differences in the variety and geographical origin of the beans, storage and processing conditions, roasting conditions, and brewing methods. An understanding of these differences can be helpful for quality control, process optimization, and also for providing information on flavors and characteristics that direct consumers to their preferred styles. In addition to the expected variation, the aroma profile for coffee is quite complex and comprised of a large number of individual analytes, creating an analytical challenge. Non-targeted chemical analysis techniques, like gas chromatography with mass spectrometry (GC-MS) and headspace solid phase micro-extraction (HS-SPME), are well-suited to address these challenges. With these methods, volatile and semi-volatile analytes were collected from the coffee samples, separated, and detected, resulting in identification and relative quantification information for hundreds of analytes. Analytes of interest do not need to be determined prior to acquisition, so the data were generally characterized to investigate the samples and their differences. Comprehensive two-dimensional gas chromatography (GC×GC) increases peak capacity and enhances S/N compared to GC, and also creates structured chromatograms. These additional analytical capabilities were explored and led to the detection of more analytes and an improved understanding of these complex samples. In this work, coffee brewed from a variety of beans was compared to investigate variations related to roast level.