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Abstract

Volatilomics, Foodomics and Fermentomics at Trace Levels: Role of Modern Untargeted Benchtop Analytical Strategies in Improving Coffee Research †

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Abstract: The characterization of complex products, such as foodstuffs or raw materials via metabolomic approaches, often referred to as "foodomics", is a modern and generally accepted strategy. As a derivative, "volatilomics", is an elegant way of correlating volatile organic compounds (VOCs) via the gas phase from the matrix with specific properties of that product, such as authenticity, quality or provenance. This is particularly relevant, as a major part of the aroma-relevant compounds, e.g., roasted coffee that belong to the VOC fraction, can be analyzed without sample contact using the headspace over the sample. A major challenge is the complexity of the enormous amount of different substances found, which often are not relevant as individual species, but rather their total "fingerprint", resulting from all amenable substances. This high-dimensional spectral information cannot be interpreted without applying powerful machine learning algorithms or chemometrics, a strategy which is generally referred to as "omics". Omics are known as holistic, full spectral analytical strategies which make use of the total information from a complex sample, e.g., a raw or roasted coffee bean, and they can be used to describe and better understand the desired aroma profiles, similarities or differences of products, as well as potential off-flavors at trace level concentrations. These data are combined with modern machine learning techniques to extract the maximum possible information from products to improve their quality and confirm authenticity. Typically, the required techniques are laboratory-based and not useable at the so-called point-of-care, which limits their use. This paper will demonstrate the principles and examples of benchtop "volatilomics" approaches in food and fermentation processes, named as "fermentomics", that be used directly at the location where they are needed in the future.

Keywords: omics; GC-IMS; foodomics; fermentomics; volatilomics

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