Beyond the “Ale” vs “Lager” paradigm in untargeted high-throughput beer chemical analysis

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Analytical technology in food and agriculture

Industrial beer quality control requires detection of subtle chemical variations between batches of the same product, yet beer represents a complex matrix which demonstrates a variety of chemical properties, depending on raw materials employed in production and the brewing process parameters. For this reason, chemical analysis on beer samples has always covered a special role as a benchmark for the development of new analytical methodologies. The wide majority of studies in this field showcases a very common sampling method, which consists of the collection of several types of commercial beer, ranging from lagers to ales, and successive measurements in triplicates [1, 2]. This setup is valid to demonstrate the analytical power of a method or data analysis technique in discriminating different beers through their chemical features, but it has several limitations for direct applicability into real-world scenarios. In the context of industrial quality control, where consistency and repeatability are key, inter- and intra-batch variability checks of the same product dominate over assessing differences among product categories [3]. For this reason, high-throughput chemical methods able to capture minute differences between batches are required [4-6].

Here, we report our learned best practices for the analysis of commercial lager beers (Carlsberg and Tuborg) through untargeted high-throughput headspace chemical analysis employing SIFT-MS, PTR-MS, and GC-MS. We demonstrate how focusing on single beer styles reveals variables such as production location that are masked when analyzing diverse beer categories and could become statistically significant indicators of variation. Additionally, we show different techniques for dynamic feature selection for untargeted chemical analysis, aimed at enhancing differences between similar batches of products. In this way, we gain mechanistic understanding on beer-specific aging processes, affecting the overall quality perception, and we enable machine-learning tasks such as classification and outlier detection for business-driven quality control decisions.