Un-targeted metabolomics for the characterization of food process flavour aromas

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Current approaches for designing and optimizing formulations and processes for manufacturing food products are constrained by limited insights into the complex and dynamic relationship between product composition and sensorial consumer perception. Hence, industrial food research and development are still driven by hypothesis-led engineering approaches and trial-and-error. Consequently, food innovation rate is low. Considerable competitive edge can be gained by adopting rapid, hypothesis-generating data-driven approaches.

Metabolomics has become a valuable data-driven, holistic approach that is able to generate novel hypotheses, identify novel biomarkers and elucidate underlying modes of action. It involves many state-of-the-art technologies including a range of separation methods coupled to accurate high resolution mass spectrometry (MS). Whereas metabolomics has been applied to biofluids and plant materials, applications in processed foods is still in its infancy, especially in relation to sensory perception. Nevertheless, recent studies have shown that holistic, data-driven approaches have great potential to identify sensory-relevant compounds (1-3). From this, it became evident that existing technologies have huge potential but need further development to obtain quantitative and robust analytical data for complex food products with a large variation in composition.

The central aim of this study is focused on the un-targeted analysis of aroma-related volatiles of yeast extract process flavours. For that purpose, the challenge lies on developing optimal headspace trapping techniques that give the most comprehensive picture and ensure an efficient and robust detection of volatiles. A number of volatile trapping techniques, such as solid phase microextraction (SPME), stir bar adsorption (e.g. Twister), and dynamic headspace (DHS) were compared for their relative values and robustness for the analysis of the volatiles of interest in a (semi)quantitative way with high dynamic range. Results showed that the techniques used differ in their efficiency in trapping the different classes of volatile compounds suggesting a need to tailor the volatile extraction technique depending on the composition of the process flavour. Methodologies will be developed which deliver robust data on sensory-relevant compounds, allow for identifying unknown (Maillard-related) compounds that contribute to the prediction of sensory attributes, and enable deeper insights into the chemical reactions.

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