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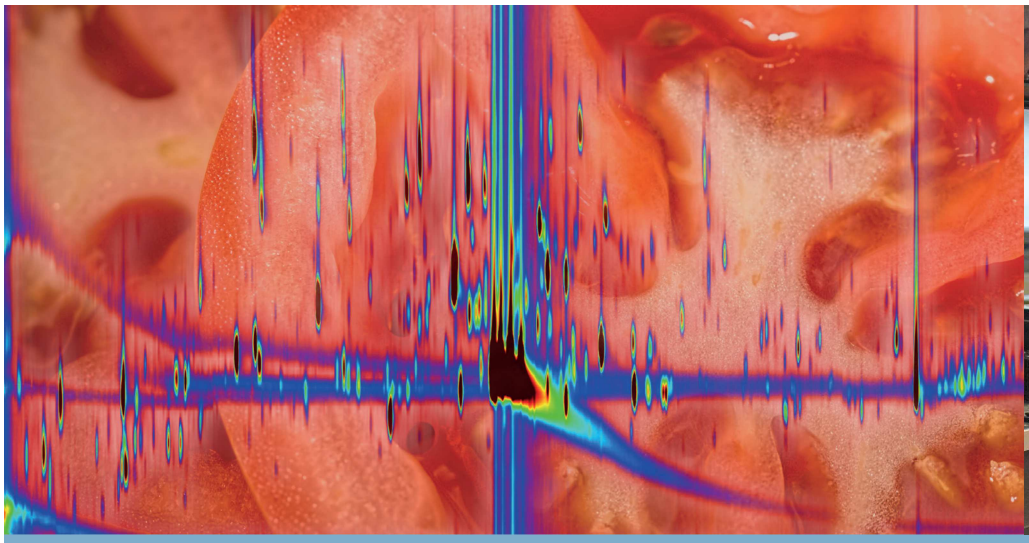

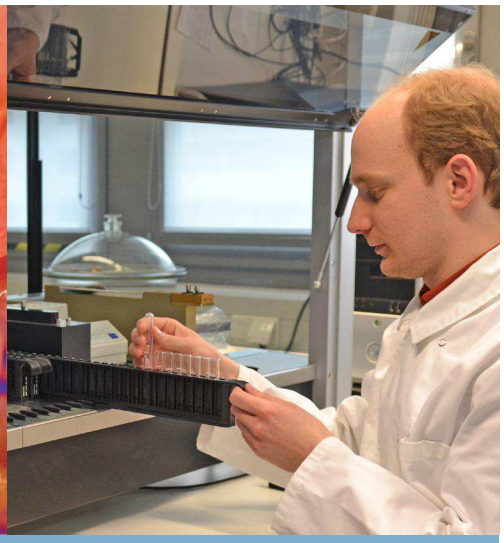

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Volatolomics by direct injection mass spectrometry

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Volatile metabolites play a relevant role in food science and technology in most, if not all, steps of the production chain: they are, e.g., important for plant ecology and physiology (plant response and signaling upon biotic or abiotic stress), they are drivers and products of fruit changes during ripening and storage and they control to a large extent the way we perceive food before (odor), during (flavour, aroma) and after (aftertaste) consumption. Moreover, being spontaneously and continuously released, volatile compounds provide a non-invasive and rapid tool for the control of food samples and the real-time monitoring of biological and technological processes.

For these reasons, the analysis of food volatolome is of interest if, mostly in an omic approach, it can provide i) high sensitivity and large dynamic range because volatile compounds can produce biological or sensory effects at different, possibly very low, concentrations and ii) fast and non-invasive measurements both to allow the screening of large sample sets and the monitoring of rapid processes.

These issues can be efficiently addressed by different Direct Injection Mass Spectrometry (DIMS) methods developed for volatile compound analysis, Proton Transfer Reaction Mass Spectrometry (PTR-MS) in particular. The lack of specificity of these techniques, as compared with chromatographic ones, is compensated by other features: they are very fast, non-invasive and provide high sensitivity even without sample pretreatment.

This contribution, after a short description of a prototypical DIMS set-up based on PTR-MS developed for agroindustrial applications, aims at pointing out DIMS pros and cons in food volatolomics by describing few selected applications investigated at the Volatile Compound Facility at FEM.

Firstly, PTR-MS profiling of berry fruit, apple and dairy products has been used for sample sets exploration and to set classification or calibration models that link food volatolome with sensory or genomics allowing, for instance, i) the efficient identification of quantitative trait loci related to fruit volatile compounds, ii) the setting of instrumental models of sensory quality which should make "sensomic" studies realistic and iii) the identification of typicality markers.

Secondly, a fully automated system for the monitoring of volatile compounds released during biological or technological processes has been developed and used to investigate microbiological processes as bread leavening, lactic and alcoholic fermentation and spoilage during storage.

Finally, DIMS allows the investigation of the interaction of food with humans or animal models, both on a sensory and health perspective, by measuring metabolites released during food consumption (nose-space analysis) or in exhaled breath (breath analysis).