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BOOK OF ABSTRACTS

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Direct injection and chromatography, mass spectrometry and ion mobility: a synergic approach for strawberry volatilome analysis

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Summary: *The aroma profiles of 15 strawberry cultivars were evaluated by PTR-ToF-MS, GC-IMS and GC-MS. The obtained results showed the complementarity of these techniques*

Keywords: *PTR-ToF-MS, GC-MS, GC-IMS*

Introduction

Strawberry quality and aroma

Flavour is one of main factors impacting strawberry quality and consumer appreciation. Since flavour involves the perception of a plethora of volatile organic compounds (VOCs), their assessment is crucial to guarantee the selection and marketability of high-quality fruits. Thus, the great impact of VOCs on fruit marketability stimulates the need to step forward in the understanding of this quality trait. High priority should be given to replace poor flavour cultivars with favourable ones, exploiting the variability already available in nature. However, the analysis of the aroma trait in many samples, necessary to overcome the usually massive biological and genetic variability among samples, may be laborious and time consuming.

VOC phenotyping is currently a limiting step in breeding programs, due to high costs and complex analytical techniques. Another limitation also raised by the elevated, and difficult to be controlled, interaction between fruit genetics and environmental effects. While there is substantial flavor variation within fruit species, most plant breeding programs have historically neglected it, given its intrinsic complexity and costs to phenotype. As a consequence, the drop-off in flavor quality has become one of the major causes of consumer dissatisfaction. To correct this inconsistency and incorporate flavor into breeding program routines, it is necessary to identify the sources of flavor variability, understand the role of genetic and environmental factors, and define cost-effective methods of selection.

Analytical techniques for VOC analysis

The most used instrumental analytical techniques for identifying volatile aroma compounds in food is gas chromatography–mass spectrometry (GC–MS). However, due to the complexity of food matrices, complicated pre-treatments generally required before analysis and long detection times this technique may not meet the rapid detection requirements for many analytes. Some complementary techniques, based on direct injection mass spectrometry (DI-

MS), have been developed to investigate VOC emissions for fruit flavor analysis, such as proton transfer reaction mass spectrometry (PTR-MS) and selected ion flow tube mass spectrometry (SIFT-MS). According to recent publications both techniques can be considered as powerful high-throughput phenotyping tool for both genetic and quality related studies [1]. The rapidity and the moderate cost of DI-MS analysis may allow to perform a detailed aroma characterization of strawberry with a peculiar attention to the VOC fold changes caused by *ad hoc* storage and transformation experiments, tailored to simulate the "from farm to fork" chain. However, a weak aspect of DI-MS methodologies for VOC assessment is still the compound identification. Fragmentation, complex peak structure and/or the presence of isomeric compounds may still make this challenge unpractical, especially in complex matrices.
Another alternative to GC-MS analysis, recently applied in food studies [2], is the application of an ion mobility spectrometry. Gas chromatography–ion mobility spectrometry (GC–IMS) combines the high separation capacity of GC and the fast response of ion mobility spectrometry (IMS). These features make GC-IMS a powerful technique for the separation and sensitive detection of VOCs in fruit and vegetables.

Experimental
In this study, the application of GC-IMS (FlavourSpec, G.A.S., Dortmund, Germany), PTR-ToF-MS (PTR-ToF-MS 8000, Ionicon, Austria) was evaluated for a comprehensive volatilome analysis on 15 strawberry cultivars. Results were compared and validated with SPME-GC-MS (AutoSystem XL gas chromatograph coupled with a TurboMass Gold mass spectrometer, Perkin-Elmer, Norwalk, CT) analysis. 9 fruits of each cultivar were firstly analysed by PTR-ToF-MS in non-destructive way (1 fruit in 250 mL jar). Then each fruit was frozen, grinned in liquid nitrogen and sampled in 20 mL vials for analysis with all three techniques.

Results
The variability of aroma profile of different cultivars was observed for all analysis. Moreover, the differences of VOC release analysed by PTR-ToF-MS between the same fruits measured as intact and grinned were also observed. The integration of four data sets were performed in the novel mixOmics framework DIABLO [3].

Conclusions
Outcomes of this study demonstrated the complementarity of three analytic methodologies and the prospect to apply them both for broad volatilome screenings and for fruit quality assessment. In particular, a proper application of these methodologies would enable, in a close future, for a more precise selection of the most favourable new accessions distinguished by superior fruit flavour, suitable for different market segments.

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