

## In-vitro and in-vivo on-line monitoring of flavour compound release during consumption of fruits from different apple cultivars

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**Summary:** Flavour profile characterization of apple cultivars is important to support fundamental research in apple physiology and genetics. This study applied Proton Transfer Reaction-Mass Spectrometry to monitor in-vitro and in-vivo flavour release of different apple cultivars. Both in-vivo and in-vitro results differentiated apple cultivars correlating flavour release, textural and physico-chemical properties.

**Keywords:** *apple (malus domestica), nose-space, PTR-MS.*

### 1 Introduction

Consumer acceptability and recognition of apple quality triggered during apple consumption arise from complex sensory sensations of olfaction, taste and trigeminal stimuli, which are perceived as odour, flavour and texture. It is reasonably expected that the release of volatile compounds during the consumption of apples is strongly influenced by the cell wall structure, which is also responsible for the perceived texture. Thus, it is clear that a proper comprehension of consumer perception of apple quality must

consider the effect of this cellular destruction during apple consumption on flavour perception.

The aim of this study was to determine the volatile compound release from six apple cultivars during in-vitro and in-vivo nose space analysis by Proton Transfer Reaction Quadrupole Mass Spectrometry (PTR-QUAD-MS) and, in particular, to investigate if flavour release during apple consumption can be monitored and if it is related to the cultivar and to other characteristics as textural properties.

### 2 Experimental

Six apple varieties were considered in this preliminary study. In-vitro static headspace measurements were carried out by PTR-QUAD-MS apparatus on whole intact apple fruit and cut apple cylinders. The in-vivo nose space analysis measured the dynamic volatile compound release from panellists ingesting, masticating and swallowing the cut apple varieties. Values of t<sub>max</sub>, time required to

reach maximum intensity (I<sub>max</sub>) and t<sub>swal</sub>, time of first swallowing event after sample ingestion were recorded. Panellists breathed into a nose piece connected to the PTR-QUAD-MS during the consumption. In addition, instrumental measurements of physico-chemical (pH, juiciness, water content and titratable acidity) and texture properties (fracturability, firmness, adhesiveness) were also analysed.

### 3 Results

The in-vitro static headspace volatile compound profiles of intact apples enabled the diverse cultivars to be differentiated. Golden Delicious, Red Delicious and Jonagold were well discriminated as clusters whereas Fuji, Granny Smith and Morgen Dallago shared similarities. This is comparable to the in-vivo

measurements. Volatile compound concentrations in the cut fruit were higher due to biochemical and enzymatic reactions occurring at the ruptured cell surfaces.

In-vivo nose space analysis showed high variability between panellists (n = 5) due to physiological differences and the application of free mastication protocols during the

experiment<sup>[1]</sup>. Four important masses were selected:  $m/z$  43, 61 ester related fragments;  $m/z$  45 acetaldehyde and  $m/z$  47 ethanol) to analyze in-vivo measurements. Concentrations of the measured volatile compounds were lower in comparison to the static headspace measurements. This was due to the interaction of released volatile compounds and immediate physico-chemical reactions occurring in the mouth during mastication as well as to the dilution of flavour compounds in the exhaled air<sup>[2]</sup>. It was however possible to identify reliable differences between the in-vivo volatile profile of each apple cultivar.

Correlation studies shown in Figure 1 showed all other cultivars were not as firm compared to Fuji and Granny Smith which were well associated with textural properties. Physico-chemical attributes of water content and acidity were positively correlated with textural properties and negatively with pH. Juiciness however, was not correlated with water content but negatively correlated with firmness and fracturability. Tmax of ester related fragments

#### 4 Conclusions

PTR-MS was demonstrated to be a useful tool for the rapid differentiation of apple cultivars by headspace analysis using whole fruits and apple disks. Nose space measurements were able to identify reliable differences between apple cultivars indicating the viability of the investigation of the complex consumer-food interaction during apple consumption. However, the in-vivo results possessed reduced signal intensities and were affected by the high variability induced by the different eating behaviour of volunteers. Apple cultivars were also well discriminated based on their flavour release, texture and physico-chemical

#### References

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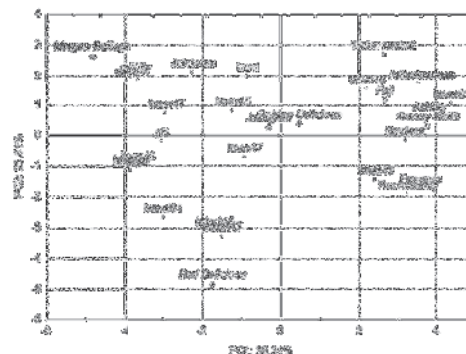


Fig. 1. First and second dimensions of PCA on the selected in-vitro and in-vivo measured flavour compounds, textural, physico-chemical properties and flavour release of cut and intact apple fruit cultivars.

( $m/z$  43, 61) were positively related and I<sub>max</sub>, negatively correlated with textural properties suggesting firmer samples had less intense ester compounds and needed more time to achieve I<sub>max</sub>. No strong correlation between intact and cut fruit signifying the importance of skin acting as a physical barrier and regulator of volatile compound diffusion.

properties providing information on the influence of structure on volatile compound profiles. Future studies will involve the use of a Proton Transfer Reaction Time of Flight Mass Spectrometer, PTR-TOF-MS, to confirm and quantify differences at higher resolution<sup>[3, 4]</sup>. This technique will allow greater chemical information to be collected, with improved time resolution that will enable a full mass spectra to be measured during nose-space measurements without the necessary pre-selection of a limited number of masses required in PTR-QUAD-MS<sup>[5]</sup>.