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Determination of Volatile Compounds in Apple bY SPME/GC-MS and Their Influence on Perceived Sweetness

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Summary: *Due the weak correlation between sugars and sweetness in apple, mass spectrometry based techniques were applied to analyze the compounds possibly linked to perceived sweetness such as sugars, acids and volatile compounds. Comparison with sweetness measured by a trained panel revealed the role of volatile compounds in sweet taste sensation enhancement.*

Keywords: *Sweetness, volatile compounds, multisensory interactions*

Introduction

It is difficult to estimate sweetness perception in apple by instrumental determinations. Sweetness correspond to the intensity of sweet taste due to the presence of simple and complex sugars and polyols and also to the multisensory process produced by the release of compounds in the mouth during food consumption. Harker found weak association between soluble solids content, fructose, glucose, saccharose, sorbitol, total sugars and sweet taste [1] and suggests the use of trained sensory panels to measure this important quality trait in apple. Sugars alone are not sufficient to explain sweetness in apple thus other factors are involved in the perception of sweet taste in apple. The interaction between sweet sensation and odours is a well-documented phenomenon [2]. In tomatoes and strawberries the role of volatile compounds in enhancing sweetness in these fruits has been proposed [3,4]. In order to improve predictability of sweetness in apple by chemical and physical determinations we decided to apply mass spectrometry based techniques to extend the analysis of compounds possibly linked with perceived sweetness such as sugars, acids and volatile compounds. A trained panel measured the sweetness of 40 batches of apple and results were compared with content of sugars (sucrose, glucose, fructose, xylose), sorbitol, malic acid, soluble solids and with volatile compounds detected by SPME/GC-MS.

Experimental

Fruits. Forty apple batches were collected during the 2013 harvesting season (more details can be found in [5]).
Sensory data. Sweetness was scored on a 0-100 scale by a trained panel of 19 assessors according the procedure reported in a previous work [6].
Chemical composition. Sugars and sorbitol were quantified by high-pressure capillary ion chromatography with pulsed amperometric detection and malic acid by UHPLC coupled with an electrospray ionization Hybrid Quadrupole-

Orbitrap Mass Spectrometer. Both methods are reported in [5]. Soluble solid content was measured in the extracted apple juice with a DBR35 refractometer (XS Instruments, Poncarale, Brescia, Italy) and are expressed as °Brix. Volatile compounds were measured by SPME/GC-MS following the procedure reported in [5].

Statistical analyses. Descriptive statistics, correlation and regression analyses were computed with the software Statistica 9.1 (StatSoft, Inc., Tulsa, OK). The software SIMCA-P+ 12.0 (Umetrics, Umeå, Sweden) was used for the building and validation of the multivariate regression models on centered and scaled (unit variance) variables.

Results

Correlation between sweetness and single sugars, total sugar amount, SSC, sorbitol and the ratios between the single sugars were weak, when significant. The parameters that better correlate to sweet taste are the sorbitol content ($p=0.661$) and SSC ($p=0.635$). Single sugars, sorbitol, SSC and malic acid were used to build an OPLS regression model. This model was able to explain no more than 60% of the sweetness of the analyzed apple. When the 95 volatile compounds identified in the headspace of apples were added to the regression model, the capacity to explain the apple sweetness increased to 92%. This clearly indicates the relevant role of volatile compounds that in synergy with sugars increase the sweetness sensation when eating apple. The major positive contributors, among volatile compounds, to sweetness are, according to the regression coefficients of the model, are the propyl 2-methylbutanoate, the propyl propanoate, the 2-methylpropyl butanoate and the 3 isomers of farnesene. The 3 esters are associated to fruity odors congruent with sweet taste perception. Farnesene is strongly correlated to esters that are developed during apple ripening [7]. On the contrary, other volatile compounds gave a negative contribution to sweetness perception in apple namely, 1-octen-3-one, 1-octen-3-ol, 6-methyl-5-hepten-2-ol, methyl butanoate, 5-hexenyl acetate, ethyl hexanoate and (Z)-3-hexen-1-ol. In this case most of them are described as not "sweet-congruent" and associated to odors like fungal or green-grass.

Conclusions

In this study, we quantified the major sugars (sucrose, glucose, fructose, xylose), sorbitol, malic acid and volatile compounds in apple and explored their influence on perceived sweetness. Our data confirm the weak correlation between sweetness and SSC. We found that sorbitol content correlates (similarly to SSC) with perceived sweetness better than any other single sugars or total sugar content and that volatile compounds are important enhancers of sweet taste in apple. The predictive OPLS model shows that after sorbitol and SSC, the most important contribution to apple sweetness is provided by several volatile compounds, mainly esters and farnesene. In conclusion, the research for increasing sweetness in apple breeding programs should take into account not only sugar content but also factors such as volatile compounds, texture parameters, minor components (i.e., polyphenols) and information from sensory panels.

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