Polyphenol analysis in horticultural products based on laser-induced fluorescence spectroscopy

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During recent years several research groups focussed on the development of non-destructive product monitoring methods to improve the process management for horticultural products in the entire supply chain. Optical methods have been applied for fruit monitoring in production and postharvest processes using mobile measuring equipment or NIR sorting lines. Besides the quality aspect of horticultural products also the demand of foodstuffs promoting a better healthiness such as functional foods has increased, due to actual discussions and new findings of the relation between nutrition and healthiness based on clinical studies. In this context fruit and vegetable became more and more popular, since they posses valuable compounds built up in the secondary metabolism. Polyphenols constitute one of the most important groups of these health promoting compounds in horticultural products. They have specific activity in the human metabolism regarding bioavailability, antioxidative capacity, interactance with enzymes and influence on gene expression. The aim of the present study was to quantitatively determine health promoting native fruit polyphenols by means of laser-induced fluorescence spectroscopy.

On different horticultural products (carrot, apple, strawberry) the fluorescence and reflectance spectra were detected, while the polyphenols contents were analyzed chromatographically for developing calibration models. The influence of side-effects (temperature, concentration) on the fluorescence signal was studied in phenol standards, fruit extracts and sliced fruit tissue. In the complex fruit matrix the quantitative determination of fruit compounds by means of fluorescence signals is influenced by the compounds' fluorescence quantum yield as well as reabsorption and quenching effects of the fruit tissue. To take these re-absorption and fluorescence quenching effects into account, partial least squares (PLS) regression has been used to built calibration models for the polyphenol analyses on the fruit fluorescence spectra (apples, strawberries) using the chromatographical analyses of phenols as a dependent variable. Different pre-processing methods such as normalization, derivation, genetic algorithms, and direct orthogonal signal correction (DOSC) have been applied to enhance the robustness of the calibration models. The uncertainty of the models was evaluated by their root mean squares errors of calibration and cross-validation. Autoscaling the spectral data along the samples and subtracting 2 DOSC factors from the matrix of, e.g., strawberry fluorescence spectra led to $r^2 = 0.98$ for the content of p-cumaroyl-glucose in the fruits.

The feasibility of the non-destructive analysis in practice is influenced by the high variability of horticultural products. To evaluate the robustness of the calibration, the models were validated on an independent test set, which leads to $r^2 = 0.94$ and rmsep = 15.03 % for the strawberries and their p-cumaroyl-glucose content. Thus, the mathematical data pre-processing method of DOSC removed the non relevant information in the spectral data and resulted in the lowest errors. In comparison, the often applied empirical approach in fluorescence spectroscopy to correct the fluorescence spectral data with the simultaneously recorded reflectance spectra to reduce re-absorption effects did not improve the calibration models. This data processing step leads to less robust models in the before mentioned example of strawberries and their p-cumaroyl-glucose content (rmsep > 55%).