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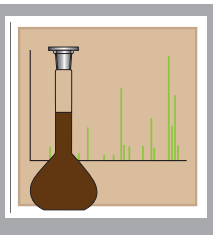

Highlights of Analytical Chemistry in Switzerland

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When Machine Tastes Coffee: Successful Prediction of Coffee Sensory Profiles by Instrumental Methods Based on On-line PTR-MS

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Flavour scientists have long been exploring what makes coffee smells so good. Analytical chemists have discovered a range of impact compounds contributing to coffee flavour, while sensory scientists have developed hedonic methods for accurate coffee flavour profiling. Although both approaches look at the same phenomenon, albeit from different perspectives, correlating instrumental data with sensory profiles has proven to be a difficult task. This is due to two fundamental challenges.

First, intensity scales in sensory and analytical measurements are of fundamentally different nature. Sensory attributes are evaluated within an arbitrary range (*e.g.* 0 to 10). In contrast, instrumental measurements result in signals that are not restricted in intensity, thus leading to very different relationships between the intensities of sensory versus analytical signals. Second, sensory scores are not proportional to concentration and each odorant follows a specific non-linear sigmoid dose–response curve. In contrast, instrumental signals are in general linear with concentration. Hence, diluting coffee by a defined factor will result in instrumental intensities reduced by the given factor leaving the signal intensity ratios unaltered. However, diluting coffee makes its sensory profile not just less intense, but may result in a flavour profile of its own.

We have succeeded to accurately predict sensory profiles of espresso coffees of different cup sizes and flavour profiles based on instrumental Proton Transfer Reaction-Mass Spectrometry (PTR-MS) data, by applying a novel chemometric strategy. Correlation was conducted according to a knowledge-based standardization of sensory and instrumental data. The key to success was a procedure removing the information of absolute intensities leading to data sets essentially containing only quality information (sensory profiles and instrumental data; green arrow in the Fig.). From here on, the correlation could be completed according to well known procedures of principle component regression (PCR).

The result is a powerful predictive tool for coffee sensory profiles (Fig. centre), applicable to short cups as well as Lungo coffees. The predictive model was validated on a set of eight additional coffees. Furthermore, the prediction of sensory profiles can be accomplished by on-line PTR-MS within two minutes.

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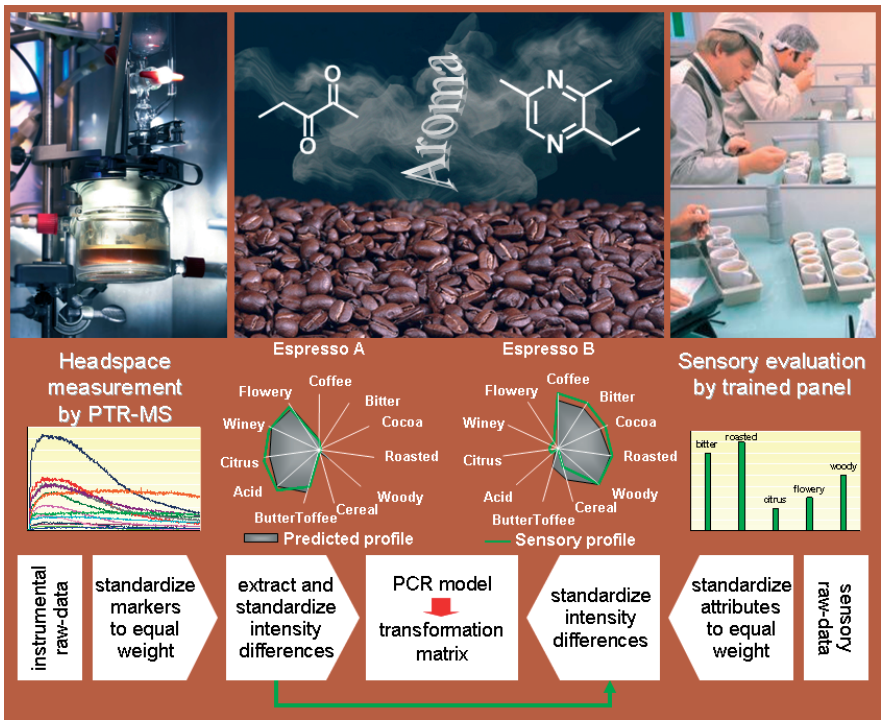
Reference

C. Lindinger, D. Labbe, P. Pollien, A. Rytz, M.-A. Juillerat, C. Yeretzian, I. Blank, *Anal. Chem.* **2008**, *80*, 1574.



Sensory predictive model: Once the sensory attributes and analytical signals are selected for maximum differentiating potential, PTR-MS data and sensory profiles are standardized to equal weight. In the case of sensory data, only a few corrections are needed since all attributes are already evaluated within an arbitrary range (0 to 10). PTR-MS data were standardized to the mean value for each individual chemical marker considering all samples. This data treatment, which is different from that of the sensory data, does not entail any limitation to a minimum or maximum value, thus allowing subsequently adding even more extreme coffee samples to the model. A knowledge-based standardization and normalization procedure of both datasets (green arrow) permits removing the information of absolute intensities and focusing on data that essentially contain only quality information. The correlation of both datasets by using PCR resulted in a robust and reproducible predictive model. Centre: Two examples of distinctively different coffees showing the sensory profiles and model results.

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