[P 051] New comprehensive procedure for enhanced data analysis and interpretation of Real-Time Measurements: A unique feature for real time flavour generation.

Monforte A R[1], Ziere A[2], Silva Ferreira A C[1], Martins S I F S[2]

1) Catholic University of Portugal, Porto, Portugal
2) Unilever R&D Vlaardingen, Vlaardingen, The Netherlands
sara.martins@unilever.com

Real-time measurements of low-abundance aroma compounds in breath from release during food consumption are already feasible due to progress in analytical technologies, such as PTR-ToF-MS. Nevertheless, the information content of real-time measurements is not fully exploited, due to the limited number of suitable data handling methods for, namely, in-vivo measurements [1]. Other software tools have been reported, but not focusing on food systems [2, 3]. This study developed a data scientific procedure to enhance flavor data analysis and interpretation from real-time studies, during food processing and consumption. The developed software addresses challenges such as mass calibration, variable number reduction and extraction of relevant masses. The developed features include 1) data projection, 2) establishment of a threshold for peak apex extraction, 3) visualization of sample expression for a specific mass, 4) application of co-clustering and principal component analysis for sample clustering exploration. These were validated for real time flavor generation in a dynamic study designed to evaluate different parameters in the formation of phenylacetaldehyde in model systems. Sequential additions of metals, glucose, gallic acid as well as sulphur dioxide have been tested. As way of example, it was observed in real time that different reaction rates for phenylacetaldehyde formation occured when metals were added in the end or in the beginning of the experiment. The developed software showed a considerable increase in efficiency of data treatment mainly in the extraction of candidate masses, capable to be contextualized for both flavor release and flavor generation as function of process conditions.

1. Szymanska E, Brown, P A, Ziere, A, Martins, S I F S, Batenburg, M, Harren, F J M, Buydens, L M C. Comprehensive Data Scientific Procedure for Enhanced Analysis and Interpretation of Real-Time Breath Measurements in In Vivo Aroma Release Studies. Anal. Chem. 2015, 87, 10338 - 10345.
2. Holzinger, R. PTRwid: A new widget tool for processing PTR-TOF-MS data. Atmos. Meas. Tech. 2015, 8, 3903 - 3922.
3. Müller, M, Mikoviny, T, Jud, W, DAnna, B, Wisthaler, A. A new software tool for the analysis of high resolution PTR-TOF mass spectra. Chemometrics and Intelligent Laboratory Systems 2013, 127, 158 - 165.