

## L-29 ANALYTICAL AND SENSORY METHODS FOR THE DETECTION OF OFF-FLAVORS

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The odor active fraction of a product (food or non-food) is normally the smallest part of the product but the most important one for accepting or rejecting it. Due to the fact that the volatile fraction can consist of a large number of different substances having different chemical structures, polarities and concentrations over several orders of magnitude makes the identification of the “key compounds” can be a really tricky game. To solve the puzzle a combination of several techniques is required to target the relevant substances. The first approach includes a multitude of sensory methods i.e. where human panelists act as analytical instruments judging the odor of a product. The second approach to odor analysis involves analytical instruments and since odor-active compounds are volatile per se, gas chromatography (GC) is the method of choice. However, no analytical instrument can deliver the most important information –whether a compound is odor-active or not. Additionally, for odor analysis several challenges have to be accounted for when employing analytical instrumentation. First, most odor-active compounds can have sensory threshold in very low concentration ranges down to the nanogram per kilogram range. Thus, one needs to develop methods which have their detection and quantification limits in the same range. This involves concentration steps and the risk of contamination and/or analyte losses. Second, in most cases the “quest” for these small concentrations is often heavily disturbed by non-odor-active volatiles which are present in several magnitudes higher concentrations, often above the maximum GC column capacity, and one has to separate these components from the compounds of interest before the GC analyses, especially when bearing in mind the needed concentration step to reach the sensory threshold values. Several examples for the successful identification of odor active substances by the combination of sensory and analytical methods will be given in the presentation.

*Keywords: Off-flavor, sensory analysis, gas chromatography-olfactometry, comprehensive GC×GC*

## L-30\* PTR-TOF-MS ANALYSIS OF FLAVOUR PROFILES: A NEW TOOL FOR CLASSIFYING APPLE CLONES

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Proton Transfer Reaction-Mass Spectrometry, in its recently developed implementation based on a time-of-flight mass spectrometer (PTR-ToF-MS) has been evaluated as a possible tool for rapid non-destructive investigation of the volatile compounds present in the flavour profile of apple cultivars and clones. Clone characterization is a cutting-edge problem in technical management and royalty application, not only for apple, aiming at unveiling real properties which differentiate the mutated individuals. We show that PTR-ToF-MS coupled with multivariate and data mining methods may successfully be employed to obtain accurate varietal and clonal physical fingerprinting. In particular, we studied the VOCs emission profile of five different clones belonging to three well known apple cultivars, such as Fuji, Golden Delicious and Gala. In all three cases we set classification models able to distinguish all cultivars and some of the clones considered in this study. Furthermore, in the case of Gala we also identified a set of compounds contributing to such clone characterization. Beside its applicative relevance, no data on the volatile profiling of apple clones are available so far; our study indicates the viability of a metabolomic approach for apple volatile compounds based on rapid PTR-ToF-MS fingerprinting.

*Keywords: proton transfer reaction-mass spectrometry, apple (malus domestica), cultivars, clones, flavour*