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**Sensorial and analytical profiling of  
orange juice and apple juice**

Development and validation of  
shelf-life prediction models



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## Analytische Chemie



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## 1 INTRODUCTION AND OBJECTIVES

In modern product development processes, newly developed products have to be tested in terms of their analytical and sensorial stability throughout the whole shelf-life partly lasting up to one year or more. A real-time storage at ambient conditions until reaching the best before date is not efficient considering the required time and commercial resources. Therefore, shelf-life studies under accelerated storage conditions are preferred to quickly obtain an estimation of the product stability. This so-called accelerated shelf-life testing (ASLT), which is typically performed by exposing the product to elevated temperatures and/or light, has become a central step in the usual product development procedure to estimate and to ensure the product stability over the minimal product shelf-life by extrapolating the findings to real-time conditions at ambient temperatures.

This study focused on fruit juices with 100 % fruit juice content containing flavouring from the named fruit (FTNF). The selected juice matrices were orange juice and apple juice. They are the most consumed fruit juices being manufactured from one type of fruit (A.I.J.N., 2016), and their compositions of volatiles are very different.

In the past, a considerable amount of data has been published on the key volatiles of orange juice (Averbeck & Schieberle, 2009; Buettner & Schieberle, 2001; Seideneck & Schieberle, 2011) and apple juice (Hey et al., 2007; Nikfardjam & Maier, 2010, 2011; Steinhaus et al., 2005). Also the molecular changes including the degradation pathways and the sensorial deterioration have been assessed during normal aging and accelerated storage for orange juice (Bielig et al., 1972; Marcotte et al., 1998; Moshonas & Shaw, 1989, 2000; Petersen et al., 1998; Tatum et al., 1975) and to a lesser extent for apple juice (Wolter, 2011; You et al., 1994). However, these studies were not intended for the application of ASLT and a subsequent development of prediction models.

Whilst for apple juice no literature data regarding storage-related prediction models were available, there are some studies for orange juice with the aim of establishing predictive statements on the basis of an ASLT approach. Petersen et al. (1998) conducted shelf-life testing with normally stored and accelerated stored orange juice and collected data for the volatile components and the sensorial impressions at the same time for a small-sized data set. The most recent investigations with the aim of fingerprinting the volatile fraction in the context of ASLT were done by Wibowo et al. (2015a) for orange juices. However, they did not pursue an integrated approach for analytical and sensorial results and even stated as conclusion that exactly this combination must be the next step.

The objective of this work was the development and establishment of science-based prediction models regarding the stability and shelf-life of orange juice and apple juice. Different stress tests should be compared with real-time storage conditions, and both analytical and sensorial aspects should be taken into account in a holistic approach. In order to achieve this goal, the ASLT was performed by collecting the sensorial profiles by quantitative descriptive analysis (QDA) and by monitoring the kinetic behaviour of volatiles by an untargeted profiling.

For the necessary evaluation and interpretation of this comprehensive set of sensorial and analytical data, an adequate strategy was newly developed in this study. As initial steps, the sensorial data and the kinetics of the volatiles were investigated independently by different complementary univariate and multivariate statistical methods with structure-discovering and structure-confirming purposes. In addition, the kinetic behaviours of the volatiles were followed and expressed by values based on the Arrhenius approach. For the final holistic prediction model, it was a very important and a particular feature of this study to combine the sensory-related and volatiles-related data for receiving evidences for an appropriate or an inappropriate use of different stress test systems in comparison to the real-time storage.