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Quality changes of pasteurised mango juice during storage. Part I: Selecting shelf-life markers by integration of a targeted and untargeted multivariate approach

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ABSTRACT

For the first time, a multivariate approach combining targeted and untargeted data was used to obtain insight into quality changes in pasteurised mango juice (cv. 'Totapuri') as a function of storage (42 °C for 8 weeks). Mango juice samples were formulated with addition of different potential precursors for different quality-related chemical reactions: ascorbic acid, citric acid and sugars. Control (diluted mango puree with water), ascorbic acid-enriched (AA_{250} and AA_{500}), citric acid-enriched (CA, CA + AA_{250} and CA + AA_{500}) and sugar-enriched (S) samples were characterised for a range of targeted quality parameters as well as for a volatile fingerprint (untargeted). Selection of shelf-life markers or quality parameters significantly changing during shelf-life was performed over all formulations as well as per mango juice formulation. Our study showed that a common trend over all formulations was observed for colour values (VID > |0.90|), while specific shelf-life markers were selected for each formulation. In acidified mango juice samples (CA, CA + AA_{250}, CA + AA_{500}), more terpene oxides were selected compared to other formulations. In ascorbic acid-enriched samples (AA_{250}, AA_{500}, CA + AA_{250}, CA + AA_{500}), furfural and ascorbic acid were significantly changing during shelf-life. It seems that the reaction pathways for compounds being formed or degraded upon shelf-life are clearly affected by the acidity level.

1. Introduction

Mango (*Mangifera indica* L.) is one of the most important tropical fruits produced in the world. According to Food and Agriculture Organization (FAO), Asia is the largest mango producer, in which India contributes for more than 35% of the world's production (FAOSTAT, 2012). Several hundreds of mango cultivars exist but only a few are commercialised. Cultivars such as 'Alphonso', 'Haden', 'Keitt', 'Kent', 'Tommy Atkins' and 'Totapuri' are known by the consumers and they vary in colour and flavour characteristics (Singh, Singh, Sane, & Nath, 2013). As a seasonal and highly perishable commodity, mango fruit is commonly processed into different products to extend its shelf-life. By applying conventional thermal treatment, such as pasteurisation, a high-acid food product (pH < 4.6) is microbiologically safe, thus can be stored at ambient temperature for a long period (Rawson et al., 2011; Silva & Gibbs, 2004). A number of thermally-treated mango products which are available in the market are mango jam, puree, nectar, juice and canned slices (Siddiq, Akhtar, & Siddiq, 2012).

However, even after processing with the aim of shelf-life extension, it is known that food product quality is not constant, or in other words, it changes continuously over time. Even for a shelf-stable product, there is a limitation in its shelf-life due to deteriorative chemical reactions determining its best-before date (Robertson, 1999). Among all quality attributes, colour is often the first characteristic consumers use to evaluate the overall product quality. Colour can indeed be used as an indicator for a range of different (bio)chemical reactions (van Boekel, 2009). Besides colour, volatile compounds can also be linked to a broad scale of chemical reactions occurring during processing and storage (Kebede et al., 2015; Perez-Cacho & Rouseff, 2008). According to several studies, different fruit juices showed a distinct rate of quality degradation during storage (Polydera, Stoforos & Taoukis, 2005; Vásquez-Caicedo, Schilling & Carle, 2007; Burdurlu & Karadeniz, 2003; Aguiló-Aguayo, Oms-Oliu, Soliva-Fortuny & Martín-Belloso, 2009; Burdurlu and Karadeniz, 2003). Consequently, it is clear that fruit juice composition plays an important role in fruit juice stability.

In evaluating food quality changes, two approaches are described in literature (Grauwet, Vervoort, Colle, Van Loey & Hendrickx, 2014). The 'targeted analytical approach' is a hypothesis-driven approach. In this approach, one or more food characteristics of interest are known a priori and thus selected as a starting point. The food characteristics can be a food attribute (e.g., colour) or a chemical compound (e.g., vitamin C).

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The analytical methods applied in this approach are specifically optimised for the full quantitative expression of the characteristics (e.g., concentration). However, when considering the complexity of food quality-related reactions, focusing on a (set of) particular chemical reaction(s) or characteristic(s) entails the risk that other important effects can be overlooked (Kebede et al., 2015).

The second approach is the 'untargeted analytical approach' (fingerprinting). This approach considers as many chemical compounds as possible and allows an initial fast screening to detect differences among samples. Since no single analytical methodology is applicable to detect, quantify and identify as much as possible analytes in a given food matrix, no matter what, a specific decision needs to be made on the food fraction to be analysed, for example either a liquid or headspace fraction of the food. Consequently, compared to the targeted approach, the untargeted approach offers a more hypothesis-free technique, however, the quantification is relative to other (control/treated) samples (e.g., relative concentration) and the identification of the unknown compounds is often a challenging task (Grauwet et al., 2014).

The objective of this work is to study the quality changes of pasteurised, shelf-stable mango juice as a function of shelf-life. Because different chemical compositions may lead to different chemical reactions, in our work, besides the control mango juice (mango puree and water), mango juice samples were formulated with addition of different potential precursors for different quality-related chemical reactions (e.g., degradation of ascorbic acid, acid-catalysed degradation of sugars): ascorbic acid, citric acid and sugars. In our previous study, these compounds were linked to changes in targeted quality parameters (e.g., colour, HMF and furfural) of pasteurised orange juice during storage at ambient and elevated temperature (Wibowo et al., 2015b; Wibowo et al., 2015c). Moreover, in the work on orange juice, fingerprinting of the volatile fraction showed potential to investigate different quality-related chemical reactions (Wibowo, Grauwet, Kebede, Hendrickx & Van Loey, 2015a). It is known that volatiles are often involved in process- and storage-induced chemical reactions and can be used as a witness for what is happening in other food fractions (e.g., liquid fraction) (Kebede et al., 2015; Vervoort et al., 2012). Also, the availability of mass spectral libraries of the GC-MS allows preliminary volatile compound identification.

In the current work, to obtain insight in the mango juice quality changes as a function of shelf-life and over the different mango juice compositions, a wide range of quality attributes were evaluated. More particular, we integrated a targeted and untargeted analytical approach, i.e., both targeted (colour, acidity, sugars, oxygen, vitamin C, furfural, HMF and carotenoids) and untargeted (volatile fraction) data were combined into one multivariate data set. In this paper or in Part I of this work, multivariate data analysis was used to find shelf-life markers or quality attributes clearly changing as a function of shelf-life. Focus is given to the higher correlation to storage time as indicated by the higher Variable Identification coefficients (VIDs). From this, a selection of shelf-life markers and their link to different reaction pathways are discussed. In the second paper or in Part II, the kinetics of the selected shelf-life markers are studied and modelled in detail.

2. Materials and methods

2.1. Experimental set-up

The experimental set-up used in this work is schematically presented in Fig. 1. Mango juice was produced as such (control) and at different formulations (Section 2.2). Juices were thermally pasteurised and stored at accelerated shelf-life conditions (42 °C) for a period of 8 weeks (Section 2.2). ASLT works on the basic assumption that the principles of chemical kinetics can be applied to quantify the effects of extrinsic parameters (e.g., temperature) on the rate of deteriorative chemical reactions (Robertson, 1999). At particular selected time moments, mango juices were sampled. As a function of shelf-life, all mango juices were characterised for a range of targeted quality parameters (Section 2.3) as well as for a volatile fingerprint (untargeted, Section 2.4). All obtained targeted and untargeted data were combined in one dataset and analysed with multivariate data analysis in order to select those quality characteristics significantly changing as a function of shelf-life (Section 2.5).

2.2. Mango juice formulation, processing and storage

Mango juice was prepared in seven different formulations; the first formulation was the control juice, which was prepared by mixing not from concentrate (NFC) mango puree cv. 'Totapuri' (16.7–17.6 °Brix) with water in 1:1 ratio (*v*/*v*). The other formulations were prepared by adding 230 mg L^{-1} and 460 mg L^{-1} ascorbic acid (AA_{250} and AA_{500}), 7.8 g L^{-1} citric acid (CA), combination of citric acid and ascorbic acid (CA + AA_{250} and CA + AA_{500}) and sugars (S) consisting 9.82 g L^{-1} of fructose, 20.39 g L^{-1} of glucose and 19.52 g L^{-1} of sucrose to the control juice. Conditions for addition of the reaction precursors (e.g., ascorbic acid, citric acid, sugars) were selected based on measured concentration of these precursors in orange juice (Wibowo et al., 2015b). For every formulation (i.e. control, AA_{250}, AA_{500}, CA, CA + AA_{250}, CA + AA_{500} and S), 40 L of mango juice mixture was pasteurised in a tubular heat exchanger at 92 °C during 30 s. After processing, 500 mL polyethylene terephthalate (PET) bottles were filled with pasteurised mango juice, including some headspace. Bottles were cooled to ambient temperature by submerging them into a circulating chlorinated water tank. For every formulation, 20 bottles were stored in temperature-controlled incubators (IPP500, Memmert, Schwabach, Germany) at 42 °C for 0, 1, 2, 4, 6 and 8 weeks protected from light. At each sampling time, all samples were transferred into smaller tubes (±30 mL), frozen in liquid nitrogen and stored at −80 °C. Prior to targeted and untargeted analyses, each sample tube was thawed in a circulating water bath at 25 °C.

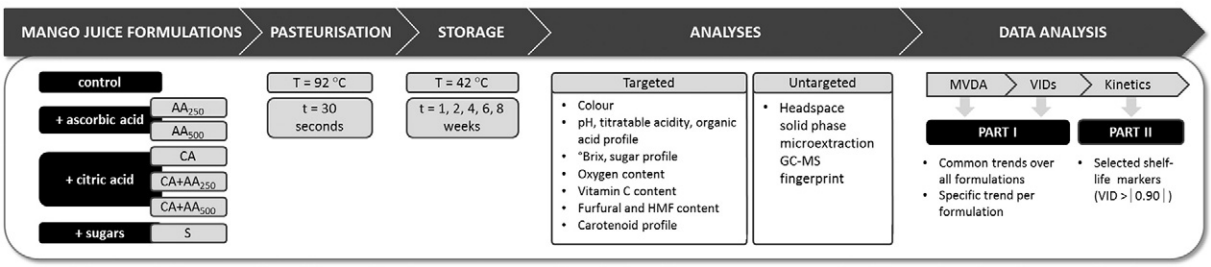

Fig. 1. Schematic overview of the mango juice experimental set-up, consisting of formulations, pasteurisation and storage conditions, list of quality parameters analysed and consecutive data analysis approach. In Part I, all obtained targeted and untargeted data were analysed by multivariate data analysis (MVDA). By the use of variable identification coefficients (VIDs), targeted quality parameters and volatiles (untargeted) clearly changing during shelf-life could be selected. In Part II, the shelf-life changes of selected markers are further zoomed into, in specific kinetic studies.