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Thermal degradation of cloudy apple juice phenolic constituents

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ABSTRACT

Although conventional thermal processing is still the most commonly used preservation technique in cloudy apple juice production, detailed knowledge on phenolic compound degradation during thermal treatment is still limited. To evaluate the extent of thermal degradation as a function of time and temperature, apple juice samples were isothermally treated during 7200 s over a temperature range of 80–145 °C. An untargeted metabolomics approach based on liquid chromatography–high resolution mass spectrometry was developed and applied with the aim to find out the most heat labile phenolic constituents in cloudy apple juice. By the use of a high resolution mass spectrometer, the high degree of in-source fragmentation, the quality of deconvolution and the employed custom-made database, it was possible to achieve a high degree of structural elucidation for the thermolabile phenolic constituents. Procyanidin subclass representatives were discovered as the most heat labile phenolic compounds of cloudy apple juice.

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1. Introduction

Despite the emerging of novel non-thermal preservation techniques, conventional thermal processing is still the most commonly used preservation technique in cloudy apple juice production (Rupasinghe & Yu, 2012). This practice is a result of its efficient inactivation of microorganisms and enzymes responsible for deterioration (Awuah, Ramaswamy, & Economides, 2007). Batch heating at 63–65 °C for 30 min. is the most traditional method (D'Amico et al., 2006). However, through the years, process optimisation was conducted by reducing processing times at high(er) temperatures in order to avoid undesirable quality changes during this process (Awuah et al., 2007). Currently, high temperature – short time (HTST) pasteurisation at 77–88 °C for 25–30 s is the most commonly used method for heat treatment of cloudy apple juice (Aguilar-Rosas, Ballinas-Casarrubias, Nevarez-Moorillon, Martin-Belloso, & Ortega-Rivas, 2007).

However, thermal processing can promote reactions that could affect colour, odour, flavour, texture and health-effect, which all could be linked to the change in phenolic profile (Niu et al., 2010). To predict the change in phenolic profile of cloudy apple juice during heat treatment, the knowledge of the phenolic composition as well as the kinetics of phenolic compound degradation, including the reaction rate as a function of temperature, are required (Vikram, Ramesh, & Prapulla, 2005).

In the past, kinetic studies regarding phenolic constituents of apple juice were mostly carried out in aqueous model solutions. For such solutions, it was already demonstrated that the heat sensitivity of phenolic compounds depends on their structure, in other words, to the phenolic subclass to which they belong (Buchner, Krumbein, Rohn, & Kroh, 2006). This tendency was confirmed in enriched apple juice during accelerated storage experiments (van der Sluis, Dekker, & van Boekel, 2005). However, it is difficult to use such intrinsic kinetic data for process optimisation given the fact that the matrix can protect against heat or promote the degradation (Ioannou, Hafsa, Hamdi, Charbonnel, & Ghoul, 2012).

Furthermore, in all available studies, only a limited set of well-known and often most abundant phenolic compounds are studied as a consequence of the employed 'targeted approach'. Following such an approach, it is very time consuming to find out the identity

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of ‘the most heat labile phenolic constituents’, while these molecules could be just the ones that are best suited to be used as ‘quality targets’ during process optimisation.

A non-targeted approach imposes itself. Due to recent technological advances in the field of High-Resolution Mass Spectrometry (HRMS), untargeted metabolomics approaches have become a feasible approach to analyse simultaneous behaviour a large amount of molecular entities in complex matrices. Therefore, the objective of the present study was to find out the most heat labile phenolic constituents in cloudy apple juice by the application of a targeted metabolomics approach. Attention will be given to the pitfalls inherent to the large-scale liquid chromatography and mass spectrometry based untargeted screening method for gathering kinetic information.

2. Materials and methods

2.1. Pilot scale cloudy apple juice production

Storage apples cv. ‘Jonagored’ (ULO storage for 10 months, caliber 65–70 mm), were purchased from a Belgian fruit auction and stored at normal atmosphere in a cold room (0 °C) until use. A combined washer/elevator/rasp mill combination (KWEM 1000, Kreuzmayr, Wallem, Germany) was used for washing and shredding the apples into mash. Subsequently, the apple mash was pressed by means of a spiral-filter pressed (VacuLIQ 1000, VacuLIQ, Hamminkeln, Germany) whereof optimised conditions were used (De Paepe, Noten, De Loose, Van Droogenbroeck, & Voorspoels, 2013). The obtained cloudy apple juice was collected in transparent plastic bags and vacuum-packed (8 mbar) just after sampling (K5N, VC999 verpackungssysteme AG, Herisau, Switzerland). Soluble solids content and pH were measured by means of digital refractometry (RM 40, Mettler-Toledo, Greifensee, Switzerland) and potentiometry (SevenCompact, Mettler Toledo, Greifensee, Switzerland), respectively.

2.2. Isothermal heat treatments

To evaluate the extent of heat treatment as a function of time and temperature, apple juice samples were isothermally treated at different time–temperature combinations. The studied temperature ranges included HTST temperatures (80, 85 and 90 °C) and ultra high temperatures (UHT, 135, 140 and 145 °C) and some temperatures in between both ranges (100 and 120 °C). To reach isothermal conditions fast, sterile capillary glass tubes (150 × 1.55 mm, VWR, Haasrode, Belgium) were used. They were filled with 150 μL of pasteurised apple juice prepared as described above and were taken through a small hole in packaging. Subsequently, each tube was brought horizontal whereby a headspace of 20 mm arose at both ends, protecting the juice for warm up during sealing. The tubes were sealed using a Bunsen burner (Sigma–Aldrich, Bornem, Belgium). Only the extreme top of the tube was brought in the flame for 1 s. For the heat treatment, the capillary tubes were completely submerged in an oil bath (Immersion circulator 1127P, VWR, Haasrode, Belgium) of which the temperature was electronically controlled. After the desired heating time (0 or untreated, 10, 20, 40, 60, 120, 300, 600, 900, 1800, 3600, 5400, and 7200 s), the tubes were removed from the oil bath and immediately cooled in ice water to stop any further reaction. The experiment as a whole (8 temperatures, 12 time points per temperature) was repeated three times on three consecutive days in a randomised block design, wherein each block represents a time series at a certain temperature.

2.3. Sample preparation

The sealed capillary tubes were degreased with 100% ethanol whereupon the tips of the tubes were broken and the samples were released in sterile tubes (Eppendorf, Nijmegen). Subsequently, the samples were centrifuged for 10 min at 12,000 rpm (13,000*g*) using a Galaxy 16DH ultracentrifuge (VWR, Leuven, Belgium). Of each obtained supernatant, 100 μL was diluted serially in a microvial by adding 150 μL U-HPLC grade methanol containing a 40 mM ammonium formate buffer. A quality control (QC) sample, assembled by pooling 20 μL of each obtained supernatant (in total 288 juice samples, coming from 3 repetitions of the eight temperatures consisting of 12 different time points), was divided into 24 aliquots and diluted in the same manner. All samples were stored at 4 °C prior to injection into the U-HPLC-DAD/ESI-am-MS system.

2.4. Analytical platform

The LC system consisted of an Accela™ quaternary solvent manager, a ‘Hot Pocket’ column oven (Thermo Fisher Scientific, Bremen, Germany) and a CTC PAL™ autosampler (CTC Analytics, Zwingen, Switzerland). A reversed phase separation was performed on a Waters Acquity UPLC™ BEH SHIELD RP18 column, with dimensions 3.0 × 150 mm, 1.7 μm (Waters, Milford, MA). To protect the U-HPLC column, an Acquity BEH C18 VanGuard pre-column, with dimensions 1.7 μm, 2.1 × 5 mm (Waters, Milford, MA) was coupled with the analytical column. The mobile phase consisted of water + 0.1% formic acid (solvent A) and acetonitrile + 0.1% formic acid (solvent B). The gradient was varied linearly from 0% to 26% B (v/v) in 9.91 min, to 65% B at 18.51 min, and finally to 100% B at 18.76 min and held at 100% B to 20.76 min. Afterwards, the initial conditions of 100% A were re-equilibrated from 20.88 min to 23.00 min prior to the next injection. The flow rate was 500 μL min^{-1} and the column temperature was set at 40 °C. Aliquots of 5 μL of the sample extract were injected into the chromatographic system. The UV spectra of all selected phenolic compounds were recorded in the range of 200–400 nm for tentative identification using an Accela™ photo diode array (PDA) detector. An Orbitrap mass spectrometer (Exactive™, Thermo Fisher Scientific, Bremen, Germany) operating with an Ion Max™ ESI source (Thermo Fisher Scientific, Bremen, Germany) in negative ionisation mode (ESI-) was used with the following operation parameters: spray voltage −2.5 kV; sheath gas (N_2, >99.99%) 47 (adimensional); auxiliary gas (N_2, >99.99%) 15 (adimensional); skimmer voltage −25 V; tube lens voltage −110 V; and capillary temperature 350 °C. The mass spectra were acquired using an acquisition function as follows: resolution, high (equivalent to a mass resolving power of 50,000 FWHM at m/z 200); automatic gain control (AGC), balanced (target value of 1×10^6), and scan speed, 2 Hz. Mass range in the full scan experiments was set at m/z 90–1800. Data acquisition and instrument control were performed using Xcalibur 2.2.1 software (Thermo Fisher Scientific, Bremen, Germany).

2.5. Measurement design

A total of 288 apple juice samples + 24 QC were analysed during two consecutive measurement series. The first measurement series consisted of the time series at the 4 lowest studied temperatures (80, 85, 90 and 100 °C), while the second measurement series consisted of the time series at the 4 highest studied temperatures (120, 135, 140 and 145 °C). Within each measurement series, the time series were measured in a randomised block design. Each time

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