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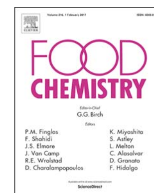

Monitoring chemical changes during food sterilisation using ultrahigh resolution mass spectrometry

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ABSTRACT

Sterilised food products undergo chemical changes during processing that ultimately determine the product quality. To provide detailed information on the chemistry of each stage of a pet-food sterilisation process, a laboratory-scale system was developed, which allowed sampling under the high temperatures and pressures associated with sterilisation. Products from the laboratory-scale system were representative of the factory process. Sample extracts were analysed by Fourier Transform-Ion Cyclotron Resonance-Mass Spectrometry (FT-ICR-MS), which delivered the molecular formulae and ion intensities of the compounds present. Data were examined to determine the coverage of this method, the degree of chemical change occurring during pet food thermal processing, and the level of identification possible with FT-ICR-MS. Data visualisation and statistical analysis identified significant chemical changes in pet food as a result of processing, and allowed tentative identification of the compounds involved. Insights generated using FT-ICR-MS analysis can be confirmed and further explored using conventional, targeted analyses.

1. Introduction

A key objective of food manufacturers is to produce consistent product quality against a background of variability in raw materials and variability in processing. Variability in raw materials may be due to seasonal or market-led factors, while variability in processing can result from factors like different manufacturing equipment in different geographical locations. Chemical changes that occur during food processing are ultimately responsible for changes in product quality attributes like nutrition, colour and flavour. The scientific literature shows that thermal processing of food initiates a wide range of sequential and interconnected chemical reactions that have historically proved difficult to unravel (see for example Davidek, Velisek, & Pokorny, 1990).

Most of the quality changes are due to the generation of reactive low molecular weight compounds (< 1000 Da) formed from naturally-occurring food components like sugars or amino acids during processing. Researchers have tended to study the reaction pathways individually, but it is well-known that significant interactions take place between products from the different pathways. An example is the production of species-specific meat flavours when the lipid oxidation and the Maillard pathways interact (Mottram, 1998). However, other chemical species like hydroxycinnamic acids can also affect the Maillard reaction (Moskowitz & Peterson, 2010) and, to gain a full picture of the chemical changes occurring in a real food during processing, it is necessary to monitor many classes of compounds. In some well-defined and well-controlled studies, flavour changes driven by the Maillard reaction have been successfully monitored. For example, aroma generation during coffee roasting in small-scale roasters was monitored as a function of the starting chemical composition and as a function of process conditions (Lindinger et al., 2008; Yeretzian, Jordan, Badoud, & Lindinger, 2002).

1.1. Processing requirements

The ambition of this study was to monitor as wide a variety of chemical compounds as possible (excluding macromolecules) during the sterilisation of a "wet" pet food. Pet food manufacture starts with the manufacture of meat chunks from animal by-products. Gravy or jelly is then added to the chunks before sterilisation at 120–130 °C for 30–60 min. Monitoring the chemical changes during the process would

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provide detailed information on the course and extent of the chemical reactions but, because the food is sealed in a can or a pouch, sampling is usually restricted to before or after processing. One way to avoid the need for direct sampling is to prepare a series of small samples in sealed glass vials and heat them for different times. Each sample is then analysed and a plot of chemical changes against sterilisation time is built from the individual data (see for example Balagiannis, Howard, Parker, Desforges, & Mottram, 2010). For large-scale experiments, this technique is laborious and time-consuming and does not allow sufficient replicates and samples to be studied to understand the variation in processing. An alternative approach is to use commercially available, small-scale pressure reactors to mimic food thermal processing and provide direct sampling during processing (Chu & Doyle, 1999; Guan, Wang, Yu, Yu, & Zhao, 2012; Hwang, Shahidi, Onodenalore, & Ho, 1997; Wang, Yang, & Song, 2012). A system that mimicked the pet food sterilisation, time-temperature profile and also allowed sampling under pressure was developed to allow the chemistry occurring during sterilisation to be studied.

1.2. Chemical analysis requirements

Assuming samples can be taken during sterilisation, the next challenge is to analyse the wide range of chemical classes present in the food, so that changes in the chemical pathways can be observed. Using conventional analytical techniques, each chemical class requires its own equipment and methods, requiring optimization, validation, replication, stability studies *etc*. Compound identification and quantification are also very time-consuming activities and, therefore, there are limits on the number of compounds that can be realistically monitored in complex systems like pet foods using conventional chemical analyses. Data processing is yet another significant task. Each analysis will provide information about changes in that particular class of compounds (e.g. in sugars, fatty acids or amino acids). It is then necessary to combine data from the different analyses in order to identify chemical reaction pathways (or relationships between compounds) from which a fundamental understanding of the chemical pathways that are taking place in the process steps could be elucidated.

Since there are parallels between the analysis of biological processes on a molecular level (metabolomics) and the analysis of chemical changes during processing, analytical methods typically used in the metabolomics area were assessed. A recent review describes the challenges needed to extract a wide range of small molecular weight, relatively polar molecules using a simple extraction procedure and an analytical system with wide compound coverage (Clark, Zhang, & Anderson, 2016). Untargeted Fourier Transform-Ion Cyclotron Resonance-Mass Spectrometry (FT-ICR-MS) was selected for this study as it allows direct infusion of sample extracts into an ion source with no chromatography, thus allowing rapid analysis and high sample throughput. Different ionisation sources can be used to optimize the analysis for the various chemical compounds, moreover, the accurate mass values obtained, allow more confident prediction of the molecular formulae, which provides a good first step towards compound identification.

Some preliminary studies on the application of high resolution mass spectrometry to food products have been published, however, they have tended to target specific chemical classes like the total and oxidised lipids in caviar (Porcari et al., 2014), checking whisky for ageing, counterfeiting and adulteration (Garcia et al., 2013), the adulteration of coffee (Garrett, Vaz, Hovell, Eberlin, & Rezende, 2012), thearubigin formation in tea (Kuhnert, Drynan, Obuchowicz, Clifford, & Witt, 2010) and vegetable oil characterisation (Wu, Rodgers, & Marshall, 2004). A preliminary study on Maillard products measured the reaction of a sugar with different amino acids in a simple model system (Golon, Kropf, Vockenroth, & Kuhnert, 2014). A comparative analysis of two cocoa bean samples was successful in identifying compounds containing CHO, CHNO and CHNO, which were identified as lipids, carbohydrates and peptides (Milev, Patras, Dittmar, Vrancken, & Kuhnert, 2014). A comprehensive study that monitored the chemical profile through the whole winemaking process, was able to identify the origin of some key wine compounds at specific processing steps, and in response to specific environmental factors, like the vineyard location and the vintage (Roullier-Gall, Lucio, Noret, Schmitt-Kopplin, & Gougeon, 2014).

1.3. Aims and objectives

The first purpose of this study was to validate a small-scale process for pet food sterilisation against the standard factory process to ensure that the same quality of product was produced in both systems. Validation used both conventional chemical and sensory analyses. The second purpose was to assess FT-ICR-MS and the data it provides. The outputs of FT-ICR-MS are accurate mass data, predicted molecular formulae and ion intensity. Molecular formulae do not provide unequivocal compound identification, as many geometric- and stereo-isomers can exist for one molecular formula. Key questions for this study were: what resolution and coverage of the varied chemical classes in pet food could be achieved; could van Krevelen diagrams (Milev et al., 2014) help visualise chemical relationships between analytes/samples and what level of compound identification could be obtained simply by accurate mass measurement? If FT-ICR-MS analysis and subsequent data processing could identify tentative identifications and chemical relationships, then conventional, targeted techniques could be applied to study these specific parts of the chemical pathways.

2. Materials and methods

2.1. Materials

All solvents (methanol, hexane, water) were HPLC grade and obtained from Sigma Aldrich (Poole, UK).

2.2. Laboratory-scale sterilisation

Sterilisation of pet food took place in a bench top reactor system (4520; Parr Instrument Company, Illinois, USA) coupled to a 4848 controller. The standard Parr steel vessel (1 L) was fitted with an electrical heating jacket, anchor-type stirring blades and a Parr sampling system. Un-sterilised product (meat chunks in gravy; typical proximate analysis moisture 84 g/100 g, protein 8.6 g/100 g, fat 4.8 g/100 g) was obtained from the local Mars Petcare factory (Melton Mowbray, UK). Two samples of the factory-sterilised product (made from the same chunk/gravy batch) were also obtained for comparative analysis. Three separate sterilisation runs were carried out, each with 800 g of un-sterilised product, which was placed in the 1 L Parr steel vessel and briefly homogenised (1 min) to avoid meat chunks blocking the sampling system. A 10-g sample was taken to represent time zero, then the vessel was closed, stirred at 6 rpm using the impeller, heated to 125 °C, held to achieve the desired f_0 value and then cooled to room temperature using ice. Samples (10 mL) were taken before and after processing (t_0 and t_6) and at five time intervals (t_1 to t_5) during the sterilisation process (using the Parr sampling system) and frozen (−18 °C) immediately. In total, 21 samples were produced for analysis, across three replicate sterilisation processes, each with seven time points between t_0 and t_6.

2.3. Validation of laboratory-scale and factory-scale processing

To ensure the fully-processed samples (t_6) from the Parr Reactor were comparable to the factory-produced product, the odour of both samples was assessed using chemical and sensory analyses. The rationale was that odour would be more sensitive to chemical changes caused by differences between the Parr and factory sterilisation

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