



# HR-CS FAAS based method for direct determination of total concentrations of Ca, Fe, Mg and Mn in functional apple beverages and evaluation of contributions of the bioaccessible fraction of these elements by in vitro gastrointestinal digestion and chemical fractionation

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## ABSTRACT

Functional apple beverages, including organic apple juices and apple juices with added species, were studied on the content of total concentrations of Ca, Fe, Mg and Mn as well as bioaccessibility of these elements and their chemical fractionation patterns. A new simplified sample preparation procedure was developed and validated for determination of Ca, Fe, Mg and Mn by high resolution-continuum source flame atomic absorption spectrometry (HR-CS FAAS). Bioaccessibility of Ca, Fe, Mg and Mn from analyzed apple beverages was assessed using in vitro simulated gastrointestinal digestion while chemical partitioning of elements species was carried out with the aid of tandem-column solid phase extraction (SPE). It was established that Ca, Mg and Mn are highly bioaccessible from functional apple beverages (> 94% of total concentrations), significantly contributing to recommended daily intakes (RDIs) of these elements, i.e. up to 11%, 19% and 21% per 1 L, respectively, for Ca, Mg and Mn.

## 1. Introduction

The quest for the healthy life style and demand for healthy and safe food have made increased consumption of natural fruit juices and functional fruit beverages. These nutritious beverages play a significant role in habitual diet of different age groups in many countries [1–6]. Apart from good taste, pleasant aroma and an exceptional nutritional value, a growing interest in these beverages is related to scientific evidence on their health benefits to humans, e.g. antioxidant and anti-inflammatory activities [1,7–9]. Fruit juices and functional fruit beverages are also an invaluable source of many essential elements that have to be considered in provision and assessment of nutrition support, primarily of infants and young children [1–5,10–16]. Regular consumption of fruit juices and functional fruit beverages can prevent many elements deficiency diseases. Conversely, their quality depends on presence of non-essential elements, e.g. heavy metals, that being in elevated amounts are harmful and even toxic [1,4,5,8,11,17]. Different environmental and non-environmental factors are responsible for a large variety in the content of minerals as well as trace elements in fruit juices and fruit beverages.

In view of food safety and nutritional considerations, it appears that

determination and control of the content of major, minor and trace elements in fruit juices and fruit beverages by atomic spectrometry methods is important and highly justified [1–5,8,14,16–19]. This is of a particular significance due to seasonal variations in quality and the chemical composition of harvested fruits [19]. On the other hand, increased consumption of fruit beverages and higher consumers' awareness about safe food products entail their more extensive production and higher nutritional safety and quality [20–22]. Popularity of commercially available fruit juices, particularly made of apples, and functional fruit beverages have also led to concern about their authenticity and origin [7,9]. A helpful approach to assessment of authenticity of fruit beverages is to reveal its element composition using appropriately fast and straightforward analytical methods and indicate differences from established reference guidelines [7,9]. Hence, development and validation of simple sample preparation procedures of fruit juices prior to their multi-element analysis by atomic spectrometry methods is of special importance. Such sample preparation procedures and analytical methods can enable faster routine element analysis of fruit juices and fruit beverages for the purpose of quality and safety control, simultaneously avoiding troublesome, prolonged and expensive high-temperature digestions with concentrated reagents.

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This is surprising but overwhelming majority of research works devoted to element analysis of fruit juices and fruit beverages do not pay any attention to speciation of elements. Research on speciation analysis of elements in fruit juices and fruit beverages in Polish and foreign literature is very scarce and inconsistent [20–22]. Usually, only available (dissolved) and bound (particulate) fractions of elements are assessed using initial samples filtration or centrifugation [23,24]. Knowledge about total concentrations of elements in fruit beverages is certainly valuable in terms of their wholesomeness and acceptability but does not provide any appreciation about functionality of elements and their bioavailability and bioaccessibility. It can be expected that speciation of elements in fruit juices and fruit beverages is complicated and have a profound effect on their bioavailability and bioaccessibility from these beverages, the uptake by the human body, and nutritional benefits. In this respect, determination of different physicochemical forms rather than the total content of essential and non-essential elements in fruit juices and fruit beverages enables to adequately evaluate their bioavailability and bioaccessibility. Nevertheless, total concentrations of elements are customarily used to compare different types of fruit juices and assess their quality and safety according to accepted regulations and guidelines. This information is also applied to estimate how the daily intake of fruit juices and fruit beverages covers recommended daily intakes (RDIs) or exceeds acceptable daily intakes (ADIs) for various elements. Such approach is not entirely justified because the actual impact of the element composition of fruit beverages on human health can differ from this anticipated on the basis of their total concentrations.

The aim of this work was to develop and validate a simplified sample preparation procedure of organic apple juices and functional apple beverages for fast sequential determination of total concentrations of Ca, Fe, Mg and Mn (nutritionally and physiologically important elements in human diet) included in them by high resolution-continuum source flame atomic absorption spectrometry (HR-CS FAAS). These essential minerals (Ca, Mg) and trace elements (Fe, Mn) were selected for the study because they are crucial for interaction between genetic and physiological factors of the body and responsible for adequate functioning of the organism at the balanced nutritional level. In addition, bioaccessibility of studied elements from mentioned organic apple juices and functional apple beverages was directly assessed by using their two-stage enzymatic digestion followed by ultrafiltration of resulting digests, simulating *in vitro* processes taking place in a gastrointestinal track. For comparison, operational speciation of Ca, Fe, Mg and Mn in analyzed organic apple juices and functional apple beverages was carried out using chemical fractionation of possible elements species with the aid of tandem-column solid phase extraction (SPE).

## 2. Material and methods

### 2.1. Equipment

An Analytik Jena AG high resolution-continuum source flame atomic absorption spectrometer (HR-CS FAAS), model *contraAA 700*, was used for fast sequential determination of Ca, Fe, Mg and Mn in all prepared solutions of samples and standards. The instrument was equipped with a xenon short-arc lamp working in a hot-spot mode and a high-resolution Echelle-type double monochromator and a charge-coupled device for detection of radiation. A sample introduction system included a PPS spray chamber with a mixing wing and an adjustable nebulizer with an Pt/Rh internal capillary and a ceramic impact bed. For delivery of solutions an AS 52 s autosampler with 87-position tray and a mixing cup for on-line “in mixing-cup” dilution was used. The whole sample introduction line was washed through 10 s after each sample/standard solution introduced into the spray chamber/pneumatic nebulizer system. A sharp air-acetylene flame operated in a Ti single-slot burner (50 mm) was used to measure all elements. Instrument settings required for flame operation were adjusted using an

**Table 1**

Operating parameters used during measurements of total concentrations of Ca, Fe, Mg and Mn by HR-CS FAAS.

	Ca	Fe	Mg	Mn
Wavelength, nm	422.7	248.3	285.2	279.5
Burner height, mm	6	6	6	6
Fuel gas (C <sub>2</sub> H <sub>2</sub> ) flow rate, L h <sup>-1</sup>	65	70	50	70
Ratio of C <sub>2</sub> H <sub>2</sub> to oxidant (air) flow rates	0.133	0.143	0.102	0.143
Spectra range (no. of pixels per spectrum)	200			
No. of pixels per signal evaluation	3			
Spectral band width, pm	2			
No. of pixels for background correction	90			
Integration time, s	3			

automatic optimization flame panel. Other parameters used were those recommended by the instrument manufacturer (see Table 1).

Absorbance was measured in an integration time mode, averaging readings within a given integration time. For calibration, 4-element simple standard solutions were prepared, covering the concentration range of 0.05–2.0 mg L<sup>-1</sup>.

Concentrations of Ca, Fe, Mg and Mn in samples solutions resulting from wet digestion of ABs was determined using an inductively coupled plasma optical emission spectrometry (ICP-OES) instrument (Agilent, model 720) with end-on observation of horizontal Ar-ICP. The spectrometer was equipped with a high-resolution Echelle-type polychromator and a VistaChip II solid-state charge-transfer device detector. Solutions of samples and standards were introduced to the ICP torch with the aid of an Agilent concentric OneNeb nebulizer, based on flow blurring nebulization technology, and a glass single-pass cyclonic spray chamber. The spectrometer was operated at standard conditions recommended by the manufacturer for solutions containing a high content of dissolved solids, i.e. forward power – 1200 W, plasma gas flow rate – 15.0 L min<sup>-1</sup>, auxiliary gas flow rate – 1.50 L min<sup>-1</sup>, nebulizing gas flow rate – 0.75 L min<sup>-1</sup>, instrument stabilization and solution uptake delay – 15 s and 30 s, respectively. Intensities of the following analytical lines were considered in quantification of elements, i.e. Ca I 422.7 nm, Fe I 248.3 nm, Mg I 285.2 nm and Mn II 257.6 nm. They were average values for 3 samplings integrated within 1 s. For calibration, 5-point calibration curves were used, spanning the concentration range of 0.01 to 5.0 mg L<sup>-1</sup>.

### 2.2. Reagents and solutions

ACS grade solutions of 65% (m/m) HNO<sub>3</sub>, 37% (m/m) HCl and 30% (m/m) H<sub>2</sub>O<sub>2</sub> were purchased from Merck (Poland). Pepsin from porcine gastric mucosa (800–2500 units per mg of protein) pancreatin from porcine pancreas, bile salts, NaCl and NaHCO<sub>3</sub> were also provided by Merck. For gastrointestinal digestion, solutions of simulated gastric (SGJ) and intestinal (SIJ) juices were freshly prepared using solid reagents. They contained 3.2 g L<sup>-1</sup> of pepsin dissolved in a mixture of 2.0 g L<sup>-1</sup> NaCl with 0.08 mol L<sup>-1</sup> HCl in case of the SGJ and 4.0 g L<sup>-1</sup> of pancreatin with 25 g L<sup>-1</sup> of bile salts dissolved in 0.1 mol L<sup>-1</sup> NaHCO<sub>3</sub> in case of the SIJ.

Merck TraceCERT single-element stock standard solutions (1000 mg L<sup>-1</sup>) of Ca, Fe, Mg and Mn were taken to prepare simple and matrix-matched (in reference to presence of HCl, SGJ and SIJ) 4-element standard solutions for calibration of HR-CS FAAS. Re-distilled water was used in all preparations.

### 2.3. Materials

Discovery DSC-18 (octadecyl groups polymerically bonded on a silica support, particle size diameter 50 μm, pore diameter 70 Å, surface area 480 m<sup>2</sup> g<sup>-1</sup>, volume 6 mL, sorbent mass 0.5 g) for reverse phase and Discovery DSC-SCX (benzene sulfonic groups polymerically bonded

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